

Page 1

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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 OCT 23 The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 4 OCT 30 CHEMLIST enhanced with new search and display field
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NEWS 6 NOV 10 CA/CAplus F-Term thesaurus enhanced
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NEWS 8 NOV 20 CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 9 DEC 01 CAS REGISTRY updated with new ambiguity codes
NEWS 10 DEC 11 CAS REGISTRY chemical nomenclature enhanced
NEWS 11 DEC 14 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 12 DEC 14 GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS 13 DEC 18 CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 14 DEC 18 CA/CAplus patent kind codes updated
NEWS 15 DEC 18 MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 16 DEC 18 MEDLINE updated in preparation for 2007 reload
NEWS 17 DEC 27 CA/CAplus enhanced with more pre-1907 records
NEWS 18 JAN 08 CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 19 JAN 16 CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 20 JAN 16 IPC version 2007.01 thesaurus available on STN
NEWS 21 JAN 16 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 22 JAN 22 CA/CAplus updated with revised CAS roles
NEWS 23 JAN 22 CA/CAplus enhanced with patent applications from India
NEWS 24 JAN 29 PHAR reloaded with new search and display fields
NEWS 25 JAN 29 CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 26 FEB 13 CASREACT coverage to be extended
NEWS 27 Feb 15 PATDPASPC enhanced with Drug Approval numbers
NEWS 28 Feb 15 RUSSIAPAT enhanced with pre-1994 records

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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DICTIONARY FILE UPDATES: 22 FEB 2007 HIGHEST RN 922553-43-3

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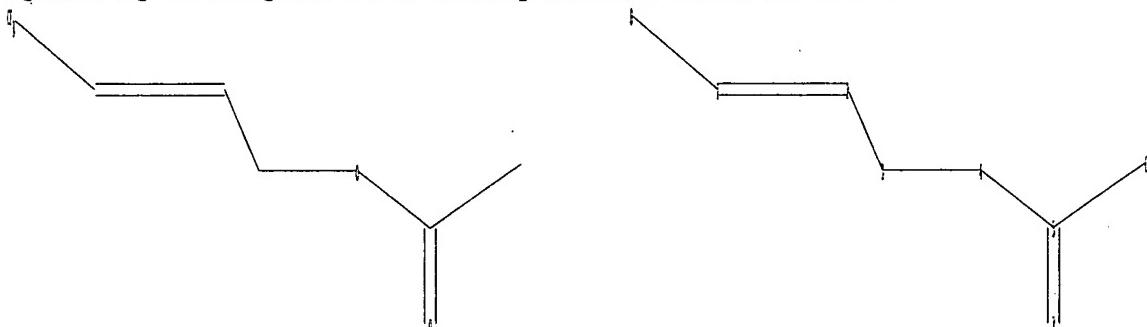
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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=>
Uploading C:\Program Files\Stnexp\Queries\10539639\Struc 3.str



chain nodes .

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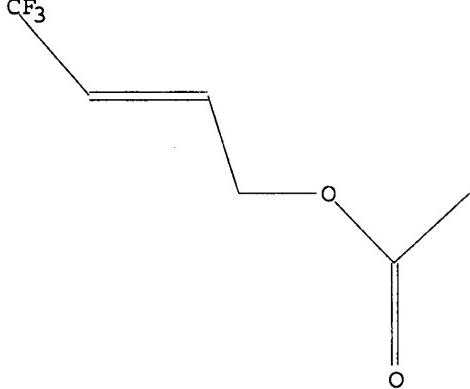
Page 3

1 2 3 4 5 6 7 8
chain bonds :
1-2 1-8 2-3 3-4 4-5 5-6 5-7
exact/norm bonds :
3-4 4-5 5-7
exact bonds :
1-2 1-8 2-3 5-6

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> l1
SAMPLE SEARCH INITIATED 15:01:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 355 TO ITERATE

100.0% PROCESSED 355 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5970 TO 8230
PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> l1 full
FULL SEARCH INITIATED 15:01:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6551 TO ITERATE

100.0% PROCESSED 6551 ITERATIONS 85 ANSWERS
SEARCH TIME: 00.00.01

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L3 85 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 172.10 172.31

FILE 'CAPLUS' ENTERED AT 15:02:01 ON 22 FEB 2007
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FILE COVERS 1907 - 22 Feb 2007 VOL 146 ISS 9
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=> l3
L4 42 L3

=> file reg
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 0.47 172.78

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DICTIONARY FILE UPDATES: 22 FEB 2007 HIGHEST RN 922553-43-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of

Page 5

experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> l1 exa

SAMPLE SEARCH INITIATED 15:02:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA EXA SAM L1

=> file caplus
COST IN U.S. DOLLARS

| | SINCE FILE ENTRY | TOTAL SESSION |
|---------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.45 | 173.23 |

FILE 'CAPLUS' ENTERED AT 15:02:32 ON 22 FEB 2007
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FILE COVERS 1907 - 22 Feb 2007 VOL 146 ISS 9
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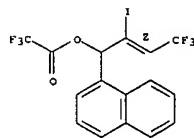
<http://www.cas.org/infopolicy.html>

=> d 14 ibib abs hitstr 1-42

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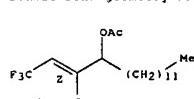
L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2006:692963 CAPLUS
 DOCUMENT NUMBER: 145:292620
 TITLE: Preparation of CF₃-containing 1,3-Di- and 1,1,3-trisubstituted allenes
 AUTHOR(S): Yamazaki, Takashi; Yamamoto, Takahiro; Ichihara, Ritsuko
 CORPORATE SOURCE: Strategic Research Initiative for Future Nano-Science and Technology, Institute of Symbiotic Science and Technology, Tokyo University of Agriculture and Technology, 2-24-16 Nakamachi, Koganei, 184-8588, Japan
 SOURCE: Journal of Organic Chemistry (2006), 71(16), 6251-6253
 CODEN: JOCHEAH ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 145:292620
 AB Novel synthetic pathway to access trifluoromethylated allenes with 1,3-di- as well as 1,1,3-trisubstitution patterns was developed from a variety of 4,4,4-trifluorobut-2-yn-1-ols which were then transformed into the corresponding vinylic iodides in highly regio- and stereospecific manners, and zinc-mediated β-elimination after trifluoroacetylation of the hydroxyl group eventually realized the formation of the target mols. in good to excellent overall yields in facile and short steps.
 IT 908608-97-9P 908608-98-0P 908609-00-7P
 908609-01-8P 908609-04-1P 908609-05-2P
 908609-07-4P 908609-08-5P 908609-09-6P
 908609-10-9P 908609-11-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of CF₃-containing 1,3-di- and 1,1,3-trisubstituted allenes from 4,4,4-trifluorobut-2-yn-1-ols)
 RN 908608-97-9 CAPLUS
 CN Acetic acid, trifluoro-, (2Z)-4,4,4-trifluoro-2-iodo-1-(1-naphthalenyl)-2-but enyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

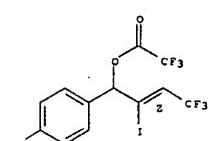


L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 908609-05-2 CAPLUS
 CN 2-Hexadecen-4-ol, 1,1,1-trifluoro-3-iodo-, acetate, (2Z)- (9CI) (CA INDEX NAME)
 Double bond geometry as shown.



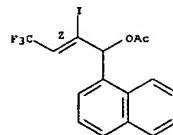
RN 908609-07-4 CAPLUS
 CN Acetic acid, trifluoro-, (2Z)-1-(4-bromophenyl)-4,4,4-trifluoro-2-iodo-2-but enyl ester (9CI) (CA INDEX NAME)
 Double bond geometry as shown.



RN 908609-08-5 CAPLUS
 CN Acetic acid, trifluoro-, (2Z)-4,4,4-trifluoro-2-iodo-1-(2-methoxyphenyl)-2-but enyl ester (9CI) (CA INDEX NAME)
 Double bond geometry as shown.

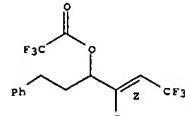
L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 908608-98-0 CAPLUS
 CN 1-Naphthalenemethanol, α-[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]-acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



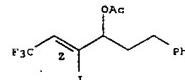
RN 908609-00-7 CAPLUS
 CN Acetic acid, trifluoro-, (2Z)-4,4,4-trifluoro-2-iodo-1-(2-phenylethyl)-2-but enyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 908609-01-8 CAPLUS
 CN Benzenepropanol, α-[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]-acetate (9CI) (CA INDEX NAME)

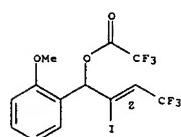
Double bond geometry as shown.



RN 908609-04-1 CAPLUS
 CN Acetic acid, trifluoro-, 1-[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]tridecyl ester (9CI) (CA INDEX NAME)

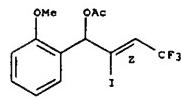
Double bond geometry as shown.

L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



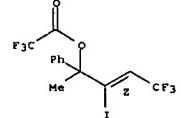
RN 908609-09-6 CAPLUS
 CN Benzenemethanol, 2-methoxy-α-[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]-acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



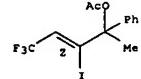
RN 908609-10-9 CAPLUS
 CN Acetic acid, trifluoro-, (2Z)-4,4,4-trifluoro-2-iodo-1-methyl-1-phenyl-2-but enyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 908609-11-0 CAPLUS
 CN Benzenemethanol, α-methyl-α-[(1Z)-3,3,3-trifluoro-1-iodo-1-propenyl]-acetate (9CI) (CA INDEX NAME)

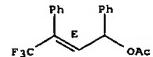
Double bond geometry as shown.



L4 ANSWER 1 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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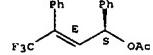
L4 ANSWER 2 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2006:283604 CAPLUS
 DOCUMENT NUMBER: 144:488118
 TITLE: Palladium-Catalyzed Regio- and Stereoselective
 Formate Reduction of Fluorine-Containing Allylic Mesylates. A
 New Entry for the Construction of a Tertiary Carbon
 Attached with a Fluoroalkyl Group
 AUTHOR(S): Konno, Tsutomu; Takehara, Tsuyoshi; Mishima, Makoto;
 Ishihara, Takashi
 CORPORATE SOURCE: Department of Chemistry and Materials Technology,
 Kyoto Institute of Technology, Kyoto, 606-8585, Japan
 SOURCE: Journal of Organic Chemistry (2006), 71(9), 3545-3550
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:488118
 AB The regioselective palladium-catalyzed formate reduction of
 γ -fluoroalkylated allylic esters is described. Reduction of the allylic
 esters under the influence of palladium with a monodentate phosphine
 ligand proceeded preferentially at the γ position, the corresponding
 reduction products with a fluoroalkyl group at the tertiary carbon being
 afforded in high yields. When the chiral allylic ester was employed,
 complete chirality transfer was observed, leading to the optically active
 materials in high yields.
 IT 887616-49-1P 887616-75-3P
 RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (palladium-catalyzed regio- and stereoselective formate reduction of
 γ -fluoroalkylated allylic esters)
 RN 887616-49-1 CAPLUS
 CN Benzenemethanol, α -[(1E)-3,3,3-trifluoro-2-phenyl-1-propenyl]-,
 acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 887616-75-3 CAPLUS
 CN Benzenemethanol, α -[(1E)-3,3,3-trifluoro-2-phenyl-1-propenyl]-,
 acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L4 ANSWER 2 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L4 ANSWER 3 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:1330461 CAPLUS
 DOCUMENT NUMBER: 144:69722

TITLE: Process for preparing 4-vinyl-2-oxo-1-pyrrolidine
 derivatives by intramolecular allylation

INVENTOR(S): Lurquin, Francoise; Driessens, Frank; Calleert,

Michel

PATENT ASSIGNEE(S): Ucb, S.A., Belg.

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXKD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

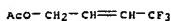
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2005121082 | A1 | 20051222 | WO 2005-EP5689 | 20050526 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
CN, CO, CR, CU, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, S2, T2, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG | | | | |
| AU 2005251884 | A1 | 20051222 | AU 2005-251884 | 20050526 |
| CA 2568700 | A1 | 20051222 | CA 2005-2568700 | 20050526 |
| PRIORITY APPLN. INFO.: | | | EP 2004-13715 | A 20040611 |
| | | | WO 2005-EP5689 | W 20050526 |

OTHER SOURCE(S): CASREACT 144:69722; MARPAT 144:69722
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

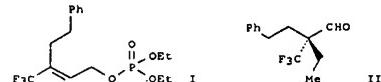
AB The present invention relates to a new process for preparing
 2-oxo-1-pyrrolidine derivs. of general formula (I) ($R_2, R_3 = H, Cl-4$
 alkyl, cyano, aryl, $-CO_2R$, halogen, R_8CO_2 , R_9SO_2O or $R_{10}SO_2O$; $R_1 = R_a$,
 R_b , C_2-20 alkenyl, aryl- C_2-20 alkenyl; $X = CONR_1R_2$, CO_2R_3 , cyano;
 $R_7-R_{10} = H$, R_a' , R_b' ; $R_11-R_{13} = H, Cl-4$ alkyl, aryl, arylalkyl,
 heteroaryl, heterocycloalkyl; $R_a, R_a' = Cl-20$ alkyl or $Cl-20$ alkyl
 substituted by one or more halogen, OH, SH, NH₂, NO₂, cyano, thiocyanato,
 CO_2H , sulfonic acid, R_b , alkylsulfonyl, arylsulfonyl, alkylsulfinyl,
 arylsulfanyl, alkylthio, arylthio, alkoxy, aryloxy, sulfonamide, acyl,
 ester, amido, N₃, acyloxy, esteroxy and/or amidoxy; $R_b, R_b' =$ each
 (un)substituted aryl, heterocycloalkyl, or heteroaryl), comprising the
 cyclization of an intermediate of general formula (II) ($R_1-R_3 =$ same as
 above; $Y =$ a leaving group selected from halogen, $-OC(O)R_4$, OSO_2R_5 ,
 etc.; R_14, R_{15} = halogen, each (un)substituted alkyl, arylalkyl, or aryl;
 X is as defined for X ; $W =$ an electron withdrawing group selected from
 CO_2R_4 , COMe, cyano, $PO(OEt)_2$, SO_2 -aryl, $-CO$ -aryl; $R_4 = H$, each

L4 ANSWER 3 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 (un)substituted Cl-6 alkyl, aryl, or arylalkyl) in the presence of one or more org. and/or inorg. bases. Thus, a soln. of compd. (IIX) (304 g) in 607 mL MeCOEt was slowly added to a soln. of DBU (179 g) in 358 mL MeCOEt under stirring in a 2 L flask at room temp. for 1 h and treated with 300 mL 1 N HCl while keeping the temp. below 25° (pH = 6-7) to give, after workup, 384 g 4-(2,2-difluorovinyl)-2-oxopyrrolidine deriv. (IV) (R = Me) (99% yield). A soln. of 77.5 g Na2CO3 in 680 mL H2O was cooled to 20° and treated with a soln. of 85 g IV (R = Me) in MeOH and the resulting mixt. was stirred at 25° for 24 h. The aq. phase was extd. with iso-Pr acetate (2 X 170 mL), and then acidified with 121 mL concd. HCl to pH = 2 while maintaining the temp. below 25°. The mixt. was then stirred at room temp. for 20 h. The solid thus obtained was filtered, washed with H2O, and then dried under vacuum to give 55 g of crude acid IV (R = H) (68% yield) which was recrystd. from methanol to give pure compd. (V) (R5 = CO2H) as a white powder (70% yield). V (R5 = CO2H) (141.9 g) was suspended in 426 mL Me iso-Bu ketone and the suspension was heated at reflux for 6 h, cooled to room temp., concd. in vacuo to give, after recrystn. from Me iso-Bu ketone 71% V (R5 = H), namely (2S)-2-[(4S)-4-(2,2-difluorovinyl)-2-oxo-1-pyrrolidinyl]butanamide.
 IT 728040-39-9, Acetic acid 4,4,4-trifluoro-2-butenyl ester
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 4-vinyl-2-oxo-1-pyrrolidine derivs. by intramol. allylation
 (cyclization) of N-[R-(leaving group)-substituted 2-butenyl]-*o*-electron withdrawing group-*o*-substituted acetamides)
 RN 728040-39-9 CAPLUS
 CN 2-Buten-1-ol, 4,4,4-trifluoro-, acetate (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 ACCESSION NUMBER: 2004:978761 CAPLUS
 DOCUMENT NUMBER: 142:113577
 TITLE: Construction of Optically Active CF3-Containing Quaternary Carbon Centers via Stereospecific SN2' Reaction
 AUTHOR(S): Kimura, Mitsu; Yamazaki, Takaishi; Kitezumi, Tomoya;
 Kubota, Toshio
 CORPORATE SOURCE: Graduate School of Bioscience and Biotechnology,
 Tokyo
 SOURCE: Institute of Technology, Midori, Yokohama, 226-8501,
 Japan
 PUBLISHER: Organic Letters (2004), 6(25), 4651-4654
 DOCUMENT TYPE: CODEN: ORLEFT; ISSN: 1523-7060
 LANGUAGE: American Chemical Society
 OTHER SOURCE(S): Journal
 English
 CASREACT 142:113577
 GI



AB Phosphates,, e.g. I, from 3-substituted 4,4,4-trifluorobut-2-en-1-ols were found to be effective for construction of CF3-containing quaternary carbon centers by way of Cu(I)-catalyzed Grignard reactions in the presence of catalytic amts. of CuCN and trimethylsilyl chloride (TMSCl) in an anti SN2' manner. Addnl., this system can be readily extended to the chiral version with the aid of BINAL-H-mediated reduction, which, by way of ozonolysis of the reaction mixture obtained, eventually realized isolation of the optically active aldehyde II with the CF3-substituted quaternary carbon center.
 IT 821799-22-8P 821799-28-4P 821799-34-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation): RACT (Reactant or reagent)
 (construction of optically active CF3-containing quaternary carbon centers via stereospecific SN2' reaction)
 RN 821799-22-8 CAPLUS
 CN 2-Penten-1-ol, 5-phenyl-3-(trifluoromethyl)-, acetate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CC(C(F)(F)C)=C(C(=O)O)C(C(F)(F)C)=C(C(F)(F)C)C(F)(F)C
 RN 821799-28-4 CAPLUS
 CN 3-Hexen-2-ol, 6-phenyl-4-(trifluoromethyl)-, acetate, (2R,3E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.

CC(C(F)(F)C)=C(C(=O)O)C(C(F)(F)C)=C(C(F)(F)C)C(F)(F)C
 RN 821799-34-2 CAPLUS
 CN 2-Buten-1-ol, 4,4,4-trifluoro-3-phenyl-, acetate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

CC(C(F)(F)C)=C(C(=O)O)C(C(F)(F)C)=C(C(F)(F)C)C(F)(F)C
 REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 ACCESSION NUMBER: 2004:609970 CAPLUS
 DOCUMENT NUMBER: 141:158947
 TITLE: Allyl esters substituted by a perfluoromethylene group, their process of synthesis and their use, and

a process for functionalizing a double bond
 INVENTOR(S): Roques, Nicolas
 PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
 SOURCE: U.S. Pat. Appl. Publ., 21 pp., Cont.-in-part of U.S. Ser. No. 203,075.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

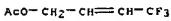
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|---|----------|--|-------------|
| US 2004147789 | A1 | 20040729 | US 2003-740802 | 20031222 |
| FR 2804955 | A1 | 20010817 | FR 2000-1744 | 20000211 |
| FR 2804955 | B1 | 20030214 | | |
| WO 2001058833 | A1 | 20010816 | WO 2001-FR364 | 20010212 |
| | N: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CY, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW | | RW: GH, GM, KE, LS, MW, MZ, SD, SL, S2, T2, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | |
| US 2003114721 | A1 | 20030619 | US 2002-203075 | 20020806 |
| FR 2849025 | A1 | 20040625 | FR 2002-16308 | 20021220 |
| FR 2849025 | B1 | 20051014 | FR 2000-1744 | A 20000211 |
| | | | WO 2001-FR364 | W 20010212 |
| | | | US 2002-203075 | A2 20020806 |
| | | | FR 2002-16308 | A 20021220 |

OTHER SOURCE(S): MARPAT 141:158947
 AB This invention provides compds. RfR1C:CR3CH2OZ, in which Rf is a radical that carries a perfluoromethylene group, which group ensures bonding to the remainder of the mol.; R1 and R3, which can be the same or different, are chosen from among hydrogen and alkyl or aryl radicals; X is an electroattractor group such that X-O-H is an acid whose pKa (in water) is at most equal to 8, advantageously 6, and preferably 5. These compds.

are useful for the synthesis of nitrogen-containing heterocyclic compds.
 IT 728040-39-9P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (allyl esters substituted by a perfluoromethylene group, their process of synthesis and their use, and a process for functionalizing a double bond)
 RN 728040-39-9 CAPLUS

L4 ANSWER 5 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CN 2-Buten-1-ol, 4,4,4-trifluoro-, acetate (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:515327 CAPLUS

DOCUMENT NUMBER: 141:53963

TITLE: Allyl esters substituted by a difluoromethylene

group,

INVENTOR(S): Saint, James Laurent; Roques, Nicolas; Bernard, Jean Marie
 PATENT ASSIGNEE(S): Rhodia Chimie, Fr.; Rhone Poulench Chimie
 SOURCE: Fr. Demande, 31 pp.
 CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|-----------------|----------------|
| FR 2849025 | A1 | 20040625 | FR 2002-16308 | 20021220 |
| FR 2849025 | B1 | 20051014 | | |
| WO 2004065347 | A1 | 20040805 | WO 2003-FR3780 | 20031217 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
CN, CO, CR, CU, C2, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MN, MW, MX, MZ, NI, NO,
NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, 2M, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD,
TG | | | |
| | AU 2003299334 | A1 | 20040813 | AU 2003-299334 |
| | EP 1631539 | A1 | 20060308 | EP 2003-799615 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK | | | 20031217 |
| | JP 2006511592 | T | 20060406 | JP 2004-567023 |
| | US 2004147769 | A1 | 20040729 | US 2003-740802 |
| | US 2006069284 | A1 | 20060330 | US 2005-539639 |
| | PRIORITY APPLN. INFO.: | | | 20050616 |
| | | | | FR 2000-1744 |
| | | | | A 20000211 |
| | | | WO 2001-FR364 | W 20010212 |
| | | | US 2002-203075 | A2 20020806 |
| | | | FR 2002-16308 | A 20021220 |
| | | | WO 2003-FR3780 | W 20031217 |

OTHER SOURCE(S): MARPAT 141:53963

AB Trans-RfR1C:CR2CH2OR3 (Rf, R1-3 = same as in I, X = halo) with a strong N base of which the assoccd. acid has pKa 212 or a N-free anionic base in polar solvents. Thus, contacting CF3CH2CHClCH2OAc with 1 equiv. diazabicycloundecene 17 h at 0° in diisopropyl ether gave 83.22% CF3CH2CHCl2OAc.

IT 705977-03-3P, trans-4,4,4-Trifluoro-2-butenoylet acetate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of allyl esters substituted by difluoromethylene groups

by dehydrohalogenation for preparation nitrogen-containing heterocycles)

RN 705977-03-3 CAPLUS

CN 2-Buten-1-ol, 4,4,4-trifluoro-, acetate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 6 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RfR1CHXR2CH2OR3 (Rf, R1-3 = same as in I, X = halo) with a strong N base of which the assoccd. acid has pKa 212 or a N-free anionic base in polar solvents. Thus, contacting CF3CH2CHClCH2OAc with 1 equiv.

L4 ANSWER 7 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:166411 CAPLUS

DOCUMENT NUMBER: 140:339049

TITLE: Trifluoromethylated vinylic and aromatic compounds from α -(trifluoromethyl)allyl alcohols

AUTHOR(S): Radix-Large, Sylvie; Kucharski, Stephanie; Langlois, Bernard R.

CORPORATE SOURCE: Laboratoire SERCOF (UMR 5181), Universite Claude

Bernard-Lyon I, Villeurbanne, 69622, Fr.

SOURCE: Synthesis (2004), (3), 456-465

CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:339049

AB α -(Trifluoromethyl)allyl alcs.. easily available from α , β -unsatd. carbonyl compds., are readily converted into γ -(trifluoromethyl)allyl thioethers, benzyl ethers, trifluoroacetates, and oxides. A Ph substituent at the γ -position to the hydroxyl function enhances their reactivity and the ease of SN2'

or SN1' substitutions, whereas a Ph ring at the α -position allows the BrF3-mediated synthesis of (trifluoromethyl)indenes. 4-Alkyl-4-methoxy-1-(trifluoromethyl)cyclohexa-2,5-dienols, readily available from 4-alkylphenols, are easily converted to 4-alkyl(trifluoromethyl)benzenes bearing a nucleophilic substituent (MeO, Cl) either on the ring or the benzylic position.

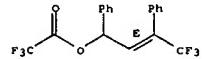
IT 681035-89-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of trifluoromethylated vinylic and aromatic compds. from α -(trifluoromethyl)allyl alcs.)

RN 681035-89-2 CAPLUS

CN Acetic acid, trifluoro-, (2E)-4,4,4-trifluoro-1,3-diphenyl-2-butenoylester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



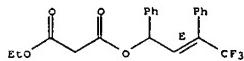
REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

Double bond geometry as shown.

L4 ANSWER 8 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:153749 CAPLUS
 DOCUMENT NUMBER: 140:374801
 TITLE: Structure determination and molecular modelling of an unexpected side product of a cyclopropane lactone formation process
 AUTHOR(S): Faigl, Ferenc; Finta, Zoltan; Heil, Zoltan; Karpati, Tamas; Harmat, Veronika; Koevesdi, Istvan; Toke, Laszlo
 CORPORATE SOURCE: Research Group for Organic Chemical Technology, Budapest University of Technology and Economics, Hungarian Academy of Sciences, Budapest, H-1521, Hung.
 SOURCE: Journal of Molecular Structure (2004), 691(1-3), 259-264
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:374801
 AB A new byproduct has been isolated from the reaction mixture of a single electron transfer induced one-pot synthesis of a cyclopropane derivative Mol. structure of the new compound has been determined by spectroscopic and single crystal X-ray diffraction methods. Formation of this indenofuran derivative has been rationalized on the basis of mol. modeling calcns. at DFT level.
 IT 283585-07-9
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (cyclization; crystallog. structure determination and potential surface modeling of an unexpected indenofuran byproduct of cyclopropane lactone formation)
 RN 283585-07-9 CAPLUS
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-diphenyl-2-butenoate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

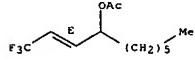
L4 ANSWER 9 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:28799 CAPLUS
 DOCUMENT NUMBER: 141:227185
 TITLE: Innovation at Rhodia Pharma Solutions. Part I - new trifluoromethylated aliphatic building blocks
 AUTHOR(S): Roques, Nicolas; Galvez, Marie; Bonnefoy, Aude; Larquetoux, Laurent; Spagnol, Michel
 CORPORATE SOURCE: Rhodia Pharma Solutions, Rhodia Inc, Cranbury, NJ, 08512-7500, USA
 SOURCE: Chimica Oggi (2003), 21(9), 43-46
 PUBLISHER: TeknoScienze
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:227185
 AB A new concept in the field of direct trifluoromethylation strategies by successfully generating in situ the "naked" trifluoromethyl anion from potassium fluoroacetate decarboxylation or trifluoromethane deprotection was introduced by Rhodia Pharma Solns. in 1995. This technol. led to the study of new industrial and economical route to potassium trifluoromethanesulfinate (CF3SO2K) and trifluoromethanesulfonyl chloride (CF3SO2Cl), which are key intermediates for the industrial production of triflic acid. The application of CF3SO2Cl as a reagent for the direct radical trifluoromethylation of simple terminal alkenes CH2=CHR', such as vinyl, allyl or isoprenyl acetate, in order to synthesize CF3CH2CHClRR' is discussed. Further basic chemical modifications of these primary precursors would lead to the production of final targeted building blocks CF3CH2-X, where X would be a reactive function (electrophile or nucleophile).
 IT 728040-39-9P
 RL: IMF (Industrial manufacture); PREP (Preparation) (manufacture of trifluoromethylated aliphatic building blocks via radical trifluoromethylation of terminal alkenes)
 RN 728040-39-9 CAPLUS
 CN 2-Buten-1-ol, 4,4,4-trifluoro-, acetate (9CI) (CA INDEX NAME)

AcO-CH2-CH=CH-CF3

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

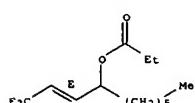
L4 ANSWER 10 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:151849 CAPLUS
 DOCUMENT NUMBER: 136:340274
 TITLE: Concise Syntheses of Nonracemic γ -Fluoroalkylated Allylic Alcohols and Amines Via an Enantioselective Palladium-Catalyzed Allylic Substitution Reaction
 AUTHOR(S): Konno, Tsutomu; Nagata, Kensuke; Ishihara, Takashi; Yamaneke, Hiroki
 CORPORATE SOURCE: Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Sakyo-Ku, Matsugasaki, Kyoto, 606-8565, Japan
 SOURCE: Journal of Organic Chemistry (2002), 67(6), 1768-1775
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:340274
 AB α -Fluoroalkylated allyl mesylates reacted with various carboxylates and amines in the presence of tetrakis(triphenylphosphine)palladium(0) catalyst to give the corresponding γ -fluoroalkylated (E)-allylic alc. derivs. and amines, resp., in excellent yields. In almost all cases, no other regio- and stereoisomers were produced. Application of this palladium-catalyzed allylic substitution reaction to various nonracemic mesylates afforded chiral γ -fluoroalkylated allylic alc. derivs. and amines without any loss of enantiomeric excess through the reaction.
 IT 320776-79-2P 320776-80-5P 320776-81-6P
 320776-82-7P 320776-91-8P 320776-94-1P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of nonracemic γ -fluoroalkylated allylic alcs. and amines via enantioselective palladium-catalyzed allylic substitution reaction)
 RN 320776-79-2 CAPLUS
 CN 2-Decen-4-ol, 1,1,1-trifluoro-, acetate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 320776-80-5 CAPLUS
 CN 2-Decen-4-ol, 1,1,1-trifluoro-, propanoate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

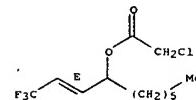


RN 320776-81-6 CAPLUS
 CN Acetic acid, chloro-, 1-[(1E)-3,3-trifluoro-1-propenyl]heptyl ester (9CI) (CA INDEX NAME)

10539639a.trn

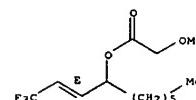
L4 ANSWER 10 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.



RN 320776-82-7 CAPLUS
 CN Acetic acid, methoxy-, 1-[(1E)-3,3-trifluoro-1-propenyl]heptyl ester (9CI) (CA INDEX NAME)

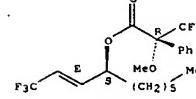
Double bond geometry as shown.



RN 320776-91-8 CAPLUS
 CN Benzenecarboxylic acid, α -methoxy- α -(trifluoromethyl)-, (1S)-1-[(1E)-3,3-trifluoro-1-propenyl]heptyl ester, (α R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

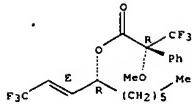


RN 320776-94-1 CAPLUS
 CN Benzenecarboxylic acid, α -methoxy- α -(trifluoromethyl)-, (1R)-1-[(1E)-3,3-trifluoro-1-propenyl]heptyl ester, (α R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

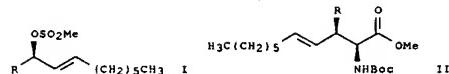
Double bond geometry as shown.

L4 ANSWER 10 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

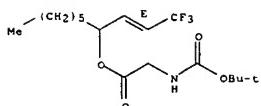
L4 ANSWER 11 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:900021 CAPLUS
 DOCUMENT NUMBER: 136:325795
 TITLE: A novel and expedient synthesis of optically active fluoroalkylated amino acids via palladium-catalyzed allylic rearrangement and Ireland-Claisen rearrangement
 AUTHOR(S): Konno, Tatsutomi; Daitoh, Takeshi; Ishihara, Takashi; Yamanaka, Hiroki
 CORPORATE SOURCE: Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Kyoto, Sakyo-ku, Matsugasaki, 606-8585, Japan
 SOURCE: Tetrahedron: Asymmetry (2001), 12(19), 2743-2748
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:325795
 GI



AB The allylic substitution reactions of various chiral α -fluoroalkylated mesylates with Boc-Gly-OH in the presence of a palladium catalyst proceeded smoothly to give γ -fluoroalkylated allyl esters in excellent yields. The esters were, then, directly subjected to Ireland-Claisen rearrangement, leading to the corresponding homochiral α -fluoroalkylated- β , γ -unsatd. amino acids in good yields. For example, fluoroalkylated mesylates I ($R = CF_3, CHF_2$) reacted with Boc-Gly-OH in an one-pot allylic substitution, followed by Ireland-Claisen rearrangement and esterification with diazomethane to give amino acid esters II.
 IT 412948-88-OP
 RL RCT (Reactant); SPP (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of optically active fluoroalkylated amino acids via palladium-catalyzed allylic substitution reaction and Ireland-Claisen rearrangement)
 RN 412948-88-0 CAPLUS
 CN Glycine, N-[[(1,1-dimethylethoxy)carbonyl]-, 1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 11 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

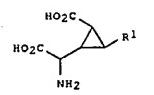


REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 12 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:881112 CAPLUS
 DOCUMENT NUMBER: 134:42439
 TITLE: Preparation of (carboxycyclopropyl)glycine derivatives
 INVENTOR(S): Collado Cano, Ivan; Pedregal Tercero, Concepcion; Marcos Llorente, Alicia; Lopez de Uralde Garnendia, Beatriz; Gonzalez Garcia, Maria Rosario; Bueno Melendo, Ana Belen
 PATENT ASSIGNEE(S): Lilly, S.A., Spain
 SOURCE: PCT Int. Appl., 132 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2000075101 | A1 | 20001214 | WO 2000-EP4903 | 20000526 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1189873 | A1 | 20020327 | EP 2000-935144 | 20000526 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| US 6498180 | B1 | 20021224 | US 2001-979322 | 20011116 |
| PRIORITY APPLN. INFO.: | | | EP 1999-500090 | A 19990603 |
| | | | WO 2000-EP4903 | W 20000526 |

OTHER SOURCE(S): MARPAT 134:42439
 GI



AB (carboxycyclopropyl)glycine derivs. I [R1 is halo-C1-10 alkyl, halo-C2-10 alkenyl, or (CH2)nY in which n is 1 or 2 and Y is OH, CN, N3, OR3, SH, S(O)pR4, SO3H, NH2, NHR5, NR6R7, NHCO8R9, NO2, CO2H, CONHR9, 1H-tetrazol-5-yl, 5-phenyltetrazol-2-yl, or PO3H2 (R3, R5, R6, R7, R8 and R9 are each selected independently from C1-4 alkyl, aryl and aryl-C1-4 alkyl; R4 is selected from C1-4 alkyl, aryl, aryl-C1-4 alkyl, 1H-tetrazol-5-yl, carboxy-C1-4 alkyl and 1H-tetrazol-5-yl-C1-4 alkyl; and P is 0-3)] or their salts or esters, provided that R1 is not

L4 ANSWER 12 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 methoxymethyl, modulate metabotropic glutamate receptor function and are useful in treating disorders of the central nervous system. Thus, (2SR,1'SR,2'RS,3'RSl)-2-(3'-hydroxymethyl-2'-carboxycyclopropyl)glycine, prepd. by a multistep procedure starting with reaction of cis-4,7-dihydro-1,3-dioxepin with Et diazoacetate, reversed [3H] LY341495 binding with a Ki of 66.1 nM at mGluR2 and 7.9 nM at mGluR3.

IT 312912-67-7P 312912-68-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (carboxycyclopropyl)glycine derivs. as excitatory

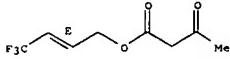
amino acid

receptor modulators)

RN 312912-67-7 CAPLUS

CN Butanoic acid, 3-oxo-, (2E)-4,4,4-trifluoro-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

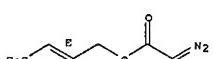


RN 312912-68-8 CAPLUS

CN Acetic acid, diazo-, (2E)-4,4,4-trifluoro-2-butenoate (9CI) (CA INDEX NAME)

NAME)

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 13 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ACCESSION NUMBER: 2000:845258 CAPLUS

DOCUMENT NUMBER: 134:115669

TITLE: Highly regio- and stereo-controlled Pd(0)-catalyzed nucleophilic substitution reaction for the synthesis of optically active γ -fluoroalkylated allylic alcohols

AUTHOR(S): Konno, Tatsutomi; Ishihara, Takashi; Yamamoto, Hiroki

CORPORATE SOURCE: Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Kyoto, 606-8585, Japan

SOURCE: Tetrahedron Letters (2000), 41(44), 8467-8472

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:115669

AB Pd(0)-catalyzed nucleophilic substitution of optically active α -(fluoroalkyl)allyl mesylates with various types of carboxylates proceeded regioselectively to afford the corresponding chiral γ -fluoroalkylated allylic alcs. in excellent yields without any loss of optical purities.

IT 320776-79-2P 320776-80-5P 320776-81-6P

320776-82-7P 320776-91-8P 320776-94-1P

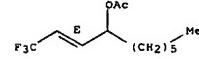
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of γ -fluoroalkyl allyl alcs. by regio- and stereoselective palladium-catalyzed nucleophilic substitution)

RN 320776-79-2 CAPLUS

CN 2-Decen-4-ol, 1,1,1-trifluoro-, acetate, (2E)- (9CI) (CA INDEX NAME)

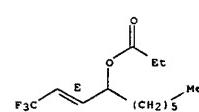
Double bond geometry as shown.



RN 320776-80-5 CAPLUS

CN 2-Decen-4-ol, 1,1,1-trifluoro-, propanoate, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

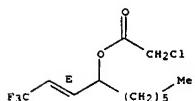


RN 320776-81-6 CAPLUS

CN Acetic acid, chloro-, 1-[(1E)-3,3,3-trifluoro-1-propenyl]heptyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

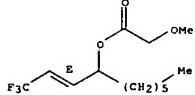
L4 ANSWER 13 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 320776-82-7 CAPLUS

CN Acetic acid, methoxy-, 1-((1E)-3,3,3-trifluoro-1-propenyl)heptyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

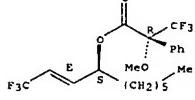


RN 320776-91-8 CAPLUS

CN Benzenoacetic acid, α -methoxy- α -(trifluoromethyl)-, (1S)-1-((1E)-3,3,3-trifluoro-1-propenyl)heptyl ester, (uR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

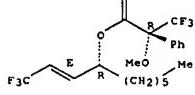


RN 320776-94-1 CAPLUS

CN Benzenoacetic acid, α -methoxy- α -(trifluoromethyl)-, (1R)-1-((1E)-3,3,3-trifluoro-1-propenyl)heptyl ester, (uR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



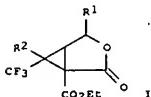
10539639a.trn

L4 ANSWER 14 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:736571 CAPLUS

DOCUMENT NUMBER: 134:42035

TITLE: Stereoselective synthesis of trifluoromethylated cyclopropanecarboxylic acid derivatives
 AUTHOR(S): Faigl, F.; Finta, Z.; Hell, Z.; DeVenyi, T.; Kovacs, I.; Toke, L.
 CORPORATE SOURCE: Szerves Kemial Technol. Tanszék, Budapesti Műszaki és Gézdaság-Tudományi Egyetem, Budapest, 1521, Hung.
 SOURCE: Magyar Kemial Polyoirat (2000), 106(9), 341-346
 CODEN: MGKPA3; ISSN: 0025-0155
 PUBLISHER: Magyar Kemikusok Egyesülete
 DOCUMENT TYPE: Journal
 LANGUAGE: Hungarian
 OTHER SOURCE(S): CASREACT 134:42035
 GI



AB Several new trifluoromethylated allylic alcs. and their monoethyl malonate

esters were prepared. These esters underwent stereoselective and, in two cases stereospecific, cyclization reactions in the presence of iodine, potassium carbonate and a phase transfer catalyst to give title compds. I (R1 = H, Me, Ph; R2 = Me, Ph). The substituents (in the allyl and vinyl positions of the starting materials) influenced the diastereoselectivity of the SET induced multistep cyclization procedure.

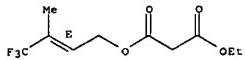
IT 197566-48-6P 197566-49-7P 197566-50-OP

283584-99-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and stereoselective cyclization of)

RN 197566-48-6 CAPLUS

CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-methyl-2-butenoylester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



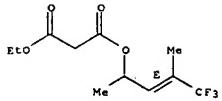
RN 197566-49-7 CAPLUS

CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-dimethyl-2-butenoylester

L4 ANSWER 14 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(9CI) (CA INDEX NAME)

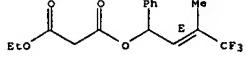
Double bond geometry as shown.



RN 197566-50-0 CAPLUS

CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-methyl-1-phenyl-2-butenoylester (9CI) (CA INDEX NAME)

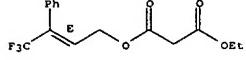
Double bond geometry as shown.



RN 283584-99-6 CAPLUS

CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-phenyl-2-butenoylester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



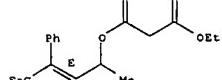
IT 283585-03-5P 283585-07-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and stereospecific cyclization of)

RN 283585-03-5 CAPLUS

CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1-methyl-3-phenyl-2-butenoylester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

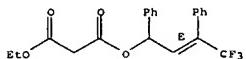


L4 ANSWER 14 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 283585-07-9 CAPLUS

CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-diphenyl-2-butenoylester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 15 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:643819 CAPLUS

DOCUMENT NUMBER: 133:335047

TITLE: First synthesis of an α -(trifluoromethyl)allenol ether via the Julia-Lythgoe process
 AUTHOR(S): Yoshimatsu, Mitsuhiro; Hibino, Masaru
 CORPORATE SOURCE: Department of Chemistry, Faculty of Education, Gifu University, Gifu, 501-1193, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (2000), 48(9), 1395-1398

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:335047

AB α -(Trifluoromethyl)allenol ethers were prepared in moderate to good yields by the Julia-Lythgoe process using β -ethoxy- β -(trifluoromethyl)vinyl Ph sulfone. Several reactions of 4-C1C6H4CH=C(C(F3)OEt) were examined to give α,β -unsatd.

IT 303734-21-6P 303734-22-7P 303734-23-8P

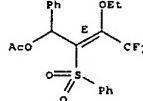
303734-24-9P 303734-25-0P 303734-26-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(first synthesis of an α -(trifluoromethyl)allenol ether via Julia-Lythgoe process)

RN 303734-21-6 CAPLUS

CN Benzenemethanol, α -(1E)-2-ethoxy-3,3-trifluoro-1-(phenylsulfonyl)-1-propenyl-, acetate (9CI) (CA INDEX NAME)

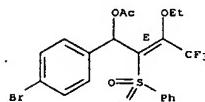
Double bond geometry as shown.



RN 303734-22-7 CAPLUS

CN Benzenemethanol, 4-bromo- α -(1E)-2-ethoxy-3,3-trifluoro-1-(phenylsulfonyl)-1-propenyl-, acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.

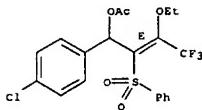


RN 303734-23-8 CAPLUS

CN Benzenemethanol, 4-chloro- α -(1E)-2-ethoxy-3,3-trifluoro-1-

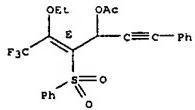
L4 ANSWER 15 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 (phenylsulfonyl)-1-propenyl-, acetate (9CI) (CA INDEX NAME)

Double bond geometry as shown.



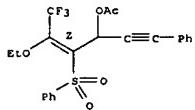
RN 303734-24-9 CAPLUS
 CN 4-Hexen-1-yn-3-ol, 5-ethoxy-6,6,6-trifluoro-1-phenyl-4-(phenylsulfonyl)-, acetate, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 303734-25-0 CAPLUS
 CN 4-Hexen-1-yn-3-ol, 5-ethoxy-6,6,6-trifluoro-1-phenyl-4-(phenylsulfonyl)-, acetate, (4Z)- (9CI) (CA INDEX NAME)

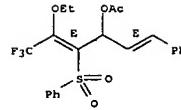
Double bond geometry as shown.



RN 303734-26-1 CAPLUS
 CN 1,4-Hexadien-3-ol, 5-ethoxy-6,6,6-trifluoro-1-phenyl-4-(phenylsulfonyl)-, acetate, (1E,4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 15 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 16 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:168918 CAPLUS

DOCUMENT NUMBER: 133:104927

TITLE: Unexpected substituent effect in the stereoselective synthesis of trifluoromethyl group containing cyclopropane lactones

AUTHOR(S): Faigl, F.; Finta, Z.; Heil, Z.; Kovacs, J.; Toke, L.
 CORPORATE SOURCE: Department of Organic Chemical Technology, Technical University of Budapest, Budapest, H-1521, Hung.
 SOURCE: Journal of Fluorine Chemistry (2000), 103(2), 117-121
 CODEN: JFLCAR; ISSN: 0022-1139

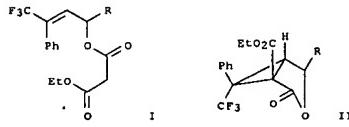
PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:104927

GI



AB Me or Ph substitution in the allylic position of malonic esters I (R = H, Me, Ph) of (E)-phenyl(trifluoromethyl)propenols resulted in unexpected and unpreceded stereospecific formation of the corresponding cyclopropane

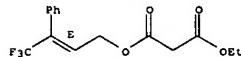
esters II by a multistep reaction with iodine in the presence of potassium carbonate and phase transfer catalyst.

IT 283584-99-6P 283585-03-5P 283585-07-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); (substituent effect in stereoselective synthesis of trifluoromethyl cyclopropane lactones by cyclization of (trifluoromethylphenylpropenyl malonates).

RN 283584-99-6 CAPLUS
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

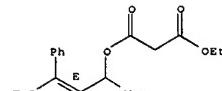


RN 283585-03-5 CAPLUS
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1-methyl-3-phenyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

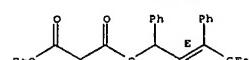
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L4 ANSWER 16 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 283585-07-9 CAPLUS
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-diphenyl-2-butene ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 17 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:736636 CAPLUS

DOCUMENT NUMBER: 131:352823

TITLE: Improved process for the preparation of trifluoromethyl containing derivatives

INVENTOR(S): Van Der Puy, Michael

PATENT ASSIGNEE(S): AlliedSignal Inc., USA

SOURCE: PCT Int. Appl., 16 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 9958488 | A1 | 19991118 | WO 1999-US10438 | 19990513 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6111130 | A | 20000829 | US 1999-307819 | 19990510 |
| AU 9939852 | A | 19991129 | AU 1999-39852 | 19990513 |
| PRIORITY APPLN. INFO.: | | | US 1998-85448P | P 19980514 |
| | | | US 1999-307819 | A 19990510 |
| | | | WO 1999-US10438 | W 19990513 |

OTHER SOURCE(S): MARPAT 131:352823

AB The present invention relates to a process for the preparation of trifluoromethylated derivs. of the formula $\text{CF}_3\text{CCl}(\text{:O})\text{R}$, wherein R is unsubstituted or substituted Cl to C6 straight chain or branched alkyl, unsubstituted or substituted C3 to C7 cycloalkyl, unsubstituted or substituted C2 to C12 alkenyl, a benzyl group unsubstituted or substituted with R', or a Ph group unsubstituted or substituted with R'; wherein R' is an unsubstituted or substituted Cl to C6 straight chain or branched alkyl; and wherein where R and/or R' are substituted each is substituted with R', by reaction of $\text{CF}_3\text{CCl}(\text{:O})\text{CH}_2\text{CH}_2\text{Cl}$ (HCFC-353) with carboxylic acid salts. The trifluoromethylated derivs., particularly $\text{CF}_3\text{CCl}(\text{:O})\text{CH}_2\text{OC(=O)CH}_3$, are versatile intermediates for the synthesis of a wide variety of trifluoromethylated organic compds. which find utility as pharmaceuticals, agricultural chems., and materials such as liquid crystals. Thus, a mixture of sodium acetate (300 g), DMF (750 mL), and HCFC-353 (323 g) were heated

L4 ANSWER 18 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:533303 CAPLUS

DOCUMENT NUMBER: 131:322201

TITLE: CuCN and trimethylsilyl chloride-catalyzed regiospecific grignard reactions to CF3-containing allylic derivs.

AUTHOR(S): Yamazaki, Takashi; Umetsu, Hideki; Kitazume, Tomoya

CORPORATE SOURCE: Department of Bioengineering, Tokyo Institute of Technology, Yokohama, 226-8501, Japan

SOURCE: Israel Journal of Chemistry (1999), 39(2), 193-205

CODEN: ISJCAT; ISSN: 0021-2148

PUBLISHER: Laser Pages Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:322201

AB CF3-containing allylic alc. derivs. were treated with an appropriate Grignard reagent in the presence of catalytic amts. of CuCN and trimethylsilyl chloride (TMSCl) to furnish products via the clean anti-SN2 mechanism. Exptl. results as well as ab initio computational analyses unambiguously demonstrated the important roles of TMSCl as a Lewis basic additive for smooth promotion of reductive elimination and inhibition of the "Cu, tpbond, F" elimination leading to undesired byproduct formation.

IT 197657-75-3 197657-84-4 197657-87-7

249283-59-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(copper cyanide and trimethylsilyl chloride-catalyzed regioselective

Grignard reaction of (trifluoromethyl)allyl derivs.)

RN 197657-75-3 CAPLUS

CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (4E)- (9CI)

(CA INDEX NAME)

Double bond geometry as shown.

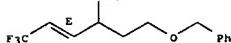


RN 197657-84-4 CAPLUS

CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (4E)- (9CI)

(CA INDEX NAME)

Double bond geometry as shown.



RN 197657-87-7 CAPLUS

CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (3S,4Z)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

10539639a.trn

L4 ANSWER 17 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
DOCUMENT NUMBER: 131:352823

TITLE: Improved process for the preparation of trifluoromethyl containing derivatives

INVENTOR(S): Van Der Puy, Michael

PATENT ASSIGNEE(S): AlliedSignal Inc., USA

SOURCE: PCT Int. Appl., 16 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

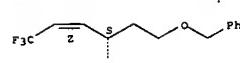
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT:

L4 ANSWER 18 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 249283-58-7 CAPLUS

CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (3R,4Z)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



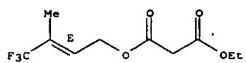
REFERENCE COUNT: 86 THERE ARE 86 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT:

FORMAT:

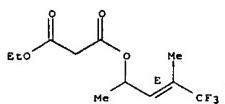
L4 ANSWER 19 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1997:635306 CAPLUS
 DOCUMENT NUMBER: 127:318840
 TITLE: Stereoselective synthesis of trifluoromethyl group containing cyclopropane lactones
 AUTHOR(S): Faigl, Ferenc; Devenyi, Tamas; Lauko, Anna; Toke, Laszlo
 CORPORATE SOURCE: Department of Organic Chemical Technology, Technical University of Budapest, Budapest, H-1521, Hung.
 SOURCE: Tetrahedron (1997), 53(38), 13001-13008
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 127:318840
 AB Malonic acid esters of trans-1-substituted-3-trifluoromethyl-2-butene-1-ols underwent stereoselective, SET induced cyclization reaction sequence in the presence of iodine, potassium carbonate and quaternary ammonium salt. The allyl substituents of the starting materials influenced the diastereoisomeric composition of the new products.
 IT 197566-48-6P 197566-49-7P 197566-50-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation): RACT (Reactant or reagent)
 (stereoselective preparation of trifluoromethyl-substituted cyclopropane lactones)
 RN 197566-48-6 CAPLUS
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-methyl-2-butenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 197566-49-7 CAPLUS
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-1,3-dimethyl-2-butenyl ester (9CI) (CA INDEX NAME)

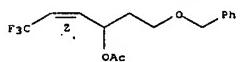
Double bond geometry as shown.



RN 197566-50-0 CAPLUS

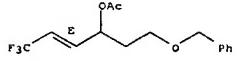
L4 ANSWER 20 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1997:626188 CAPLUS
 DOCUMENT NUMBER: 127:318689
 TITLE: Highly stereoselective SN2' reactions of Grignard reagents towards CF3-containing allylic acetates
 AUTHOR(S): Yamazaki, Takashi; Umetani, Hideki; Kitazume, Tomoya
 CORPORATE SOURCE: Dep. Bioeng., Tokyo Inst. Technol., Yokohama, 226, Japan
 SOURCE: Tetrahedron Letters (1997), 38(38), 6705-6708
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 127:318689
 AB γ -Trifluoromethylated allylic acetates were found to quite smoothly proceed SN2' type reaction with various Grignard reagents in the presence of a catalytic amount of CuCN and TMS-Cl, without any trace amount of the corresponding SN2 products in all cases examined due to the electronic effect of a CF3 group.
 IT 197657-75-3 197657-84-4
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (stereoselective SN2' reactions of Grignard reagents towards CF3-containing allylic acetates)
 RN 197657-75-3 CAPLUS
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 197657-84-4 CAPLUS
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



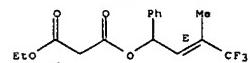
IT 197657-87-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (stereoselective SN2' reactions of Grignard reagents towards CF3-containing allylic acetates)
 RN 197657-87-7 CAPLUS
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-1-(phenylmethoxy)-, acetate, (3S,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10539639a.trn

L4 ANSWER 19 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 CN Propanedioic acid, ethyl (2E)-4,4,4-trifluoro-3-methyl-1-phenyl-2-butenoylester (9CI) (CA INDEX NAME)

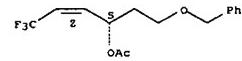
Double bond geometry as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

FORMAT

L4 ANSWER 20 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 Double bond geometry as shown.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

FORMAT

L4 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:26204 CAPLUS

DOCUMENT NUMBER: 126:74346

TITLE: Highly Stereoselective Synthesis of Trifluoromethylated Compounds via Ester-Enolate [2,3]-Wittig and [3,3]-Ireland-Claissen Rearrangements

AUTHOR(S): Konno, Tatsuharu; Umetani, Hideki; Kitazume, Tomoya

CORPORATE SOURCE: Department of Bioengineering, Tokyo Institute of Technology, Yokohama, 226, Japan

SOURCE: Journal of Organic Chemistry (1997), 62(1), 137-150

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB γ -Trifluoromethylated propryglic alcs. have been obtained in optically pure forms via effective enzymic kinetic resolution and then converted into (E)- or (Z)-allylic alcs. [2,3]-Wittig rearrangement of the corresponding γ -(trifluoromethyl)allyl]oxyacetic acid Me esters afforded α -hydroxy- β -(trifluoromethyl)- γ , δ -unsatd. carboxylic acid Me esters in good yields. The rearrangement of (Z)-substrates proceeded in highly stereoselective manner to give anti-isomers with E configuration at a newly created olefinic bond via complete chirality transfer. (E)-Substrates, however, showed relatively low stereoselectivities resulting in mixts. of syn- and anti-products. The trifluoromethylated allylic alcs. were also converted into the corresponding α -methoxyacetic acid γ -(trifluoromethyl)allyl esters and evaluated as substrates for [3,3]-Ireland-Claissen rearrangement. (E)-Substrates were efficiently transformed into syn-products while (Z)-substrates exhibited relatively low stereoselectivities. The two complementary methods provide facile routes to highly functionalized trifluoromethyl-containing mols. with a high degree of stereocontrol.

IT 185424-09-9P 185424-06-0P 185424-07-1P
185424-08-2P 185424-09-3P 185424-10-6P
185424-11-7P 185424-12-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(stereoselective synthesis of trifluoromethylated compds. via ester-enolate [2,3]-Wittig and [3,3]-Ireland-Claissen rearrangements)

RN 185424-05-8 CAPLUS

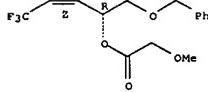
CN Acetic acid, methoxy-,

4,4,4-trifluoro-1-[(phenylmethoxy)methyl]-2-butene

ester, (R-(Z))- (9CI) (CA INDEX NAME)

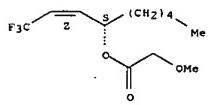
Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



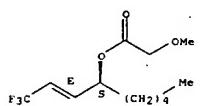
L4 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



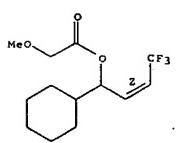
RN 185424-10-6 CAPLUS
CN Acetic acid, methoxy-, 1-(3,3,3-trifluoro-1-propenyl)hexyl ester,
[S-(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 185424-11-7 CAPLUS
CN Acetic acid, methoxy-, 1-cyclohexyl-4,4,4-trifluoro-2-butene, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 185424-12-8 CAPLUS
CN Acetic acid, methoxy-, 1-cyclohexyl-4,4,4-trifluoro-2-butene, (E)- (9CI) (CA INDEX NAME)

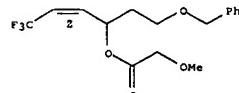
Double bond geometry as shown.

L4 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 185424-06-0 CAPLUS

CN Acetic acid, methoxy-, 4,4,4-trifluoro-1-(2-(phenylmethoxy)ethyl)-2-butene, (Z)- (9CI) (CA INDEX NAME)

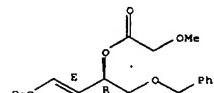
Double bond geometry as shown.



RN 185424-07-1 CAPLUS

CN Acetic acid, methoxy-, 4,4,4-trifluoro-1-(phenylmethoxy)methyl]-2-butene, [R-(E)]- (9CI) (CA INDEX NAME)

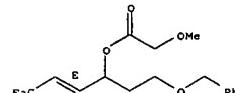
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 185424-08-2 CAPLUS

CN Acetic acid, methoxy-, 4,4,4-trifluoro-1-(2-(phenylmethoxy)ethyl)-2-butene, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

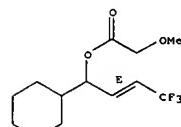


RN 185424-09-3 CAPLUS

CN Acetic acid, methoxy-, 1-(3,3,3-trifluoro-1-propenyl)hexyl ester, [S-(Z)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

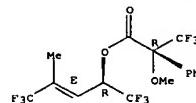
L4 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 22 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1996:693204 CAPLUS
 DOCUMENT NUMBER: 126:103713
 TITLE: Palladium(II)-catalyzed exchange and isomerization reactions. XVI The kinetics and stereochemistry of the oxidation and isomerization of hexafluoro allylic alcohols in aqueous solution catalyzed by PdCl₃(pyridine)⁻
 AUTHOR(S): Francis, John W.; Henry, Patrick M.
 CORPORATE SOURCE: Department of Chemistry, Loyola University of Chicago,
 Chicago, IL, 60626, USA
 SOURCE: Journal of Molecular Catalysis A: Chemical (1996), 112(3), 317-326
 CODEN: JMCAF2; ISSN: 1381-1169
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 126:103713
 AB Further mechanistic studies on the PdCl₃(pyridine)⁻ catalytic system in aqueous solution are described using the tetrasubstituted allylic alc., (E)-2-methyl-d₃-4-methyl-1,1,1,5,5-hexafluoro-3-penten-2-ol, 3a, and the trisubstituted allylic alc., (E)-4-Methyl-1,1,1,5,5-hexafluoro-3-penten-2-ol, 6, as substrates. At low [Cl⁻] the PdCl₁₄₂₋ catalyzed isomerization of 3a, which can only undergo isomerization into its allylic isomer, was previously found to obey the Wecker rate expression: k₁[PdCl₁₄₂₋][3a]/[H⁺][Cl⁻]². In contrast, the rate expression for isomerization of 3a by PdCl₃(Py)⁻ at low [Cl⁻] was found to be: rate = k₁[PdCl₃(Py)⁻][3a]/[Cl⁻]¹. This rate expression is of the same form as that previously found for the isomerization of 3a by PdCl₁₄₂₋ at high [Cl⁻]. This result strongly suggests that the hydronium palladation by PdCl₃(Py)⁻ at low [Cl⁻] is a trans process as opposed to a cis process with PdCl₁₄₂₋. This expectation was confirmed by stereochem. studies with chiral 3a. The stereochem. of addition for PdCl₃(Py)⁻ was identical to that for PdCl₁₄₂₋ at high [Cl⁻]. Independent stereochem. studies have shown this addition to be trans. With PdCl₃(Py)⁻ there are two possible routes for olefin oxidation. A cis process similar to that found for PdCl₁₄₂₋ or a trans process analogous to that previously proposed to explain the trans stereochem. found at high [Cl⁻]. Stereochem. studies with 6, which can undergo oxidation, showed that both processes are operative with PdCl₃(Py)⁻ at [Cl⁻] = 0.05 M. Thus addition of a pyridine to the coordination sphere of Pd(II) causes a profound change in reactivity.
 IT 185951-43-3P 185951-44-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (kinetics and stereochem. of oxidation and isomerization of aqueous hexafluoro allylic alcs. catalyzed by PdCl₃(pyridine)⁻)

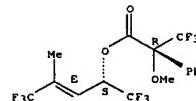
L4 ANSWER 22 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 185951-43-3 CAPLUS
 CN Benzenoacetic acid, α -methoxy- α -(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(trifluoromethyl)-2-butenoylester, [R-[R¹,R²-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



RN 185951-44-4 CAPLUS
 CN Benzenoacetic acid, α -methoxy- α -(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(trifluoromethyl)-2-butenoylester, [S-[R¹,S²-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

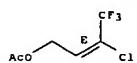


L4 ANSWER 23 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1996:661096 CAPLUS
 DOCUMENT NUMBER: 125:300456
 TITLE: Preparation of chlorotrifluorobutenes as synthetic intermediates
 INVENTOR(S): Van Der Puy, Michael
 PATENT ASSIGNEE(S): Alliedsignal Inc., USA
 SOURCE: PCT Int. Appl., 16 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|------------------|------------|
| WO 9628104 | A1 | 19960919 | WO 1996-US2963 | 19960301 |
| W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, GB, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TT, UA, UG, UZ, VN | | | | |
| RW: BE, LS, MM, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| US 5654473 | A | 19970805 | US 1995-405312 | 19950316 |
| AU 9651357 | A | 19961002 | AU 1996-51357 | 19960301 |
| EP 915066 | A1 | 19980107 | EP 1996-907923 | 19960301 |
| EP 915066 | B1 | 20000105 | | |
| RU, ES, FR, GB, IT | | | | |
| JP 11501922 | T | 19990216 | JP 1996-527678 | 19960301 |
| TW 393451 | B | 20000611 | TW 1996-85103302 | 19960321 |
| PRIORITY APPLN. INFO.: | | | US 1995-405312 | A 19950316 |
| | | | WO 1996-US2963 | W 19960301 |

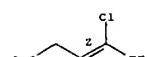
OTHER SOURCE(S): MARPAT 125:300456
 AB CF₃CCl₁:CHCH₂R (R = H, F, Br, Iodo, OH, OAc) were prepared. Thus, CF₃CCl₁ was added to CH₂:CH₂ and the product treated with Cr₂O₃ to give CF₃CCl₁:CHCH₂Cl, which was treated with KOAc to give CF₃CCl₁:CHCH₂OAc.
 IT 175401-09-9P 175401-10-2P
 RL: IMP (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of chlorotrifluorobutenes as synthetic intermediates)
 RN 175401-09-9 CAPLUS
 CN 2-Buten-1-ol, 3-chloro-4,4,4-trifluoro-, acetate, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



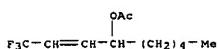
RN 175401-10-2 CAPLUS
 CN 2-Buten-1-ol, 3-chloro-4,4,4-trifluoro-, acetate, (E)- (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 Double bond geometry as shown.



L4 ANSWER 24 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1996:271988 CAPLUS
 DOCUMENT NUMBER: 125:57876
 TITLE: Stereochemical control in the silyl triflate-mediated Claisen rearrangement of allylic esters
 AUTHOR(S): Kobayashi, Masataka; Masumoto, Katsuhiro; Nakai, Ei-ichi; Nakai, Takeshi
 CORPORATE SOURCE: Dep. Chem. Technol., Tokyo Inst. Technol., Tokyo, 152, Japan
 SOURCE: Tetrahedron Letters (1996), 37(17), 3005-8
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 125:57876

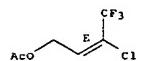
AB The titled Claisen modification proceeded with a remarkably high level of diastereoselection and asym. transmission by virtue of the proper choice of the combination of the silyl triflate and the tertiary amine used.
 IT 178251-42-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereochem. control in the silyl triflate-mediated Claisen rearrangement of allylic esters)
 RN 178251-42-8 CAPLUS
 CN 2-Nonen-4-ol, 1,1,1-trifluoro-, acetate (9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1996:106832 CAPLUS
 DOCUMENT NUMBER: 124:260321
 TITLE: Preparation, fluorination and synthetic utility of a CFC-olefin adduct
 AUTHOR(S): Van der Puy, Michael; Demmin, Timothy R.; Bindu Madhavan, G. V.; Thenappan, Alagappan; Tung, Harry S.
 CORPORATE SOURCE: AlliedSignal Inc., Buffalo Research Laboratory, 20 Peabody Street, Buffalo, NY, 14210, USA
 SOURCE: Journal of Fluorine Chemistry (1996), 76(1), 49-54
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:260321

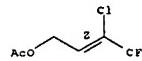
AB 1,1,1-Trifluorotrifluoroethane was added to ethylene using the catalyst system Fe/triethyl phosphite, which eliminated the need for a solvent and avoided the corrosion problems inherent in CuCl-catalyzed reactions. The adduct, CF3CCl2CH2CH2Cl, was fluorinated with HF over a chromium(III) oxide catalyst. A series of alternating dehydrochlorinations and HF addns. to internal C:C double bonds was proposed and supported by thermodyn. calcns. to explain the formation of CF3CF2CH:CH2 as the principal fluorination product. An intermediate, CF3CCl:CHCH2Cl, formed cleanly by dehydrochlorination of the adduct in the absence of HF, was converted into 4,4,4-trifluorobutanol and other compds. of the type CF3CCl:CHCH2X (X = OAc, OH, Br, I, H).
 IT 175401-09-9P 175401-10-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, fluorination, and synthetic utility of a CFC-olefin adduct)
 RN 175401-09-9 CAPLUS
 CN 2-Buten-1-ol, 3-chloro-4,4,4-trifluoro-, acetate, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

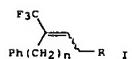


RN 175401-10-2 CAPLUS
 CN 2-Buten-1-ol, 3-chloro-4,4,4-trifluoro-, acetate, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 26 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994:298199 CAPLUS
 DOCUMENT NUMBER: 120:298199
 TITLE: Synthesis of γ -trifluoromethylated primary allylic amines
 AUTHOR(S): Felix, Caroline; Laurent, Andre; Lebideau, Frank;
 Mison, Pierre
 CORPORATE SOURCE: Lab. Chim. Org., Univ. Claude Bernard-Lyon I,
 Villeurbanne, 69622, Fr.
 SOURCE: Journal of Chemical Research, Synopses (1993), (10), 389
 CODEN: JRPSCD; ISSN: 0308-2342
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 120:298199
 GI

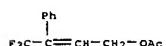


AB Preparation of trifluoromethylated primary allylic amines, e.g., Ph(CH2)n(CF3):CHCH2NH2 was achieved starting from alcs., Ph(CH2)n(CF3):(OH)CH:CH2 (I, n = 0,1,2). I was converted to the azide derivative I' (R = N3) by mesylation with mesyl chloride in CH2Cl2 followed by treatment with Na3N in DMF. Reduction of azide I' (R = N3) by PPh3/H2O gave

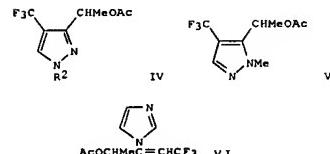
allylic amine I (R = NH2) as mixts. of E and Z isomers. Allylic amines I (R = NH2) were converted to amides I' (R = NHCOPh) by NET3-PhCOCl in CH2Cl2.

IT 154841-07-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 154841-07-3 CAPLUS
 CN 2-Buten-1-ol, 4,4,4-trifluoro-3-phenyl-, acetate (9CI) (CA INDEX NAME)



L4 ANSWER 27 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1993:560183 CAPLUS
 DOCUMENT NUMBER: 119:160183
 TITLE: Fluorinated acetylenes. Part 8. Preparation and some reactions of 5,5,5-trifluoropent-3-yn-2-ol, 5,5,5-trifluoro-1-phenylpent-3-yn-2-ol and the derived
 AUTHOR(S): Sibous, Lakhdar; Tipping, Anthony E.
 CORPORATE SOURCE: Chem. Dep., Univ. Manchester Inst. Sci. Technol., Manchester, M60 1QD, UK
 SOURCE: Journal of Fluorine Chemistry (1993), 62(1), 39-49
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 119:160183
 GI



AB Treatment of CF3C.tpbond.Cli with the aldehydes RCH2CHO (R = H and Ph) affords the secondary alcs. CF3C.tpbond.CC(H)R.OH [R1 = Me (I) and R1 = CH2Ph (II)]. I, does not give the corresponding ketone on attempted oxidation (pyridinium chlorochromate or Na2Cr2O7/H2SO4), but alc. II is oxidized to the diketone CF3C.tpbond.CCOCHPhCHPhCO.tpbond.CCF3 (41%) by

active MnO2. The acetate CF3C.tpbond.CCMeOAc (III) undergoes facile reaction with diazomethane to give [(acetoxymethyl)trifluoromethyl]pyrazoles IV (R2 = H) and hence [(acetoxymethyl)methyl(trifluoromethyl)pyrazoles IV (R2 = Me) and V, resp. Cycloaddn. also takes place between III and turan, but the major products (considered to be isomeric 1:1 adducts) have

not been fully characterized. Although, III undergoes reaction with trifluoronirosomethane, a cycloadduct has not be isolated, while nucleophilic attack by imidazole on the triple bond leads to the (Z)-alkene VI.

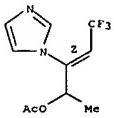
IT 149978-99-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 149978-99-4 CAPLUS
 CN 1H-Imidazole-1-ethanol, α -methyl- β -(2,2,2-trifluoroethylidene)-, acetate (ester), (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 27 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)



L4 ANSWER 28 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:489692 CAPLUS

DOCUMENT NUMBER: 117:89692

TITLE: Palladium(II)-catalyzed exchange and isomerization reactions. 15. Kinetics and stereochemistry of the isomerization of 2-(methyl-d3)-4-methyl-1,1,1,5,5-hexafluoro-3-penten-2-ol in aqueous solution

catalyzed

by PdCl42- at high chloride concentrations

Francis, John W.; Henry, Patrick M.

Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA

Organometallics (1992), 11(8), 2832-6

CODEN: ORGND7; ISSN: 0276-7333

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The isomerization of 2-(methyl-d3)-4-methyl-1,1,1,5,5-hexafluoro-3-penten-2-ol (2a) into an equilibrium mixture of 2a and

2-methyl-4-(methyl-d3)-

1,1,1,5,5-hexafluoro-3-penten-2-ol (2b) in aqueous solution was

studied by 1H

and 2H NMR spectroscopy under conditions of high chloride (>2.0 M)

concentration used previously in the presence of CuCl2 to determine the stereochemistry of hydroxypalladation. The rate expression under these conditions is rate = $k_1[PdCl42-][2a]/[Cl^-]$, with $k_1 = 1.1 \times 10^{-3} \text{ s}^{-1}$. This rate expression at high chloride concns. is identical to the rate expression found for the nonoxidative isomerization of allyl alc. under the same reaction conditions and is consistent with an equilibrium π -complex formation followed by trans attack of water to give the oxypalladation

intermediate, which reverses the process to give exchange. The fact that the attack is from outside the coordination sphere of the palladium(II) explains the single-chloride inhibition. Stereochem. studies were conducted with chiral (E)-2a. The observed result was the formation of chiral 2b with

the same configuration as the initial 2a but with the Z geometric configuration. This result is also consistent only with trans hydroxypalladation. The result also agrees with earlier stereochem. studies at high chloride concns. which used quite a different technique. The important point is that since the exchange stereochem. studies carried

out in the previous paper of this series showed the hydroxypalladation to have stereochem. opposite from that at high chloride concns., the previous stereochem. studies at high [Cl⁻] are not a valid indication of the stereochem. at low [Cl⁻].

IT 142484-36-4P

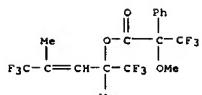
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and resolution of)

RN 142484-36-4 CAPLUS

CN Benzenoacetic acid, α -methoxy- α -(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(methyl-d3)-1-(trifluoromethyl)-2-butenoylester, (R-[R',R''-(E)])- (9CI) (CA INDEX NAME)

L4 ANSWER 28 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

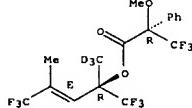
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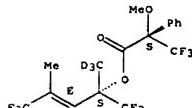
IT 135708-35-9P 142508-62-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 135708-35-9 CAPLUS

CN Benzenoacetic acid, α -methoxy- α -(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(methyl-d3)-1-(trifluoromethyl)-2-butenoylester, (R-[R',R''-(E)])- (9CI) (CA INDEX NAME)Absolute stereochemistry.
Double bond geometry as shown.

RN 142508-62-1 CAPLUS

CN Benzenoacetic acid, α -methoxy- α -(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(methyl-d3)-1-(trifluoromethyl)-2-butenoylester, (S-[R',R''-(E)])- (9CI) (CA INDEX NAME)Absolute stereochemistry.
Double bond geometry as shown.

L4 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:632522 CAPLUS

DOCUMENT NUMBER: 115:232522

TITLE: Synthesis of cis-configurated bis(trifluoromethyl)pyrethroids

AUTHOR(S): Rothermel, Reinfried; Hanack, Michael

CORPORATE SOURCE: Inst. Org. Chem., Univ. Tuebingen, Tuebingen, D-7400, Germany

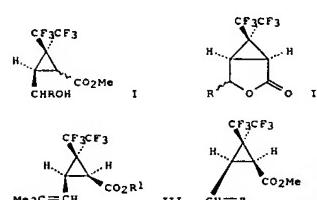
SOURCE: Liebigs Annalen der Chemie (1991), (10), 1013-20

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 115:232522

GI

AB trans-2,2-Bis(trifluoromethyl)cyclopropanecarboxylates I ($R = Me_2CH$, H) are converted into the cis-diastereomers by base-catalyzed epimerization via the bicyclic lactones II. Dehydration of cis-I ($R = Me_2CH$) and cleavage of the ester function leads to the fluorinated chrysanthemic acidIII ($R_1 = H$), which is converted into the pyrethroids III [$R = CH_2CH_2Ph_3$, $CH(CN)CH_2Ph_3$]. cis-I ($R = H$) is oxidized by pyridinium chlorochromate to give Me cis-3-formyl-2,2-bis(trifluoromethyl)cyclopropanecarboxylate (hexafluorocaronaldehydeic acid Me ester; IV; $Z = O$). This compound, which is very sensitive to isomerization, is converted into the pyrethrroid esters IV ($Z = C(CF_3)_2CH_2$) predominantly retaining the cis configuration; however, by introducing the 2,2-dichlorovinyl side chain the trans diastereomer is obtained. The starting materials trans-I are prepared by the reaction of aldehydes $AcOCH_2CHO$ ($R_2 = Me_2CH$, H) with $CF_3CCl_2CF_3$ and PPH_3 followed by cyclopropanization of the resulting 1,1-bis(trifluoromethyl)olefins, $AcOCH_2CH_2C(CF_3)_2$, with (ethoxycarbonylmethylene)dimethylsulfurane, $Me_2S:CHCO_2Et$.

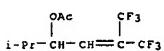
IT 121618-14-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclopropanation of, with (ethoxycarbonylmethylene)dimethylsulfurane)

RN 121618-14-2 CAPLUS

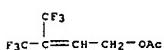
CN 4-Hexen-3-ol, 6,6,6-trifluoro-2-methyl-5-(trifluoromethyl)-, acetate (9CI)

L4 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 135524-49-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 135524-49-1 CAPLUS
CN 2-Buten-1-ol, 4,4,4-trifluoro-3-(trifluoromethyl)-, acetate (9CI) (CA INDEX NAME)



L4 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ACCESSION NUMBER: 1991:582350 CAPLUS
DOCUMENT NUMBER: 115:182350

TITLE: Palladium(II)-catalyzed exchange and isomerization reactions. 14. Kinetics and stereochemistry of the isomerization and water exchange of

2-(methyl-d3)-4-methyl-1,1,5,5-hexafluoro-3-penten-2-ol in aqueous solution catalyzed by PdCl42-. Two new mechanistic probes for catalytic chemistry Francis, John W.; Henry, Patrick M.
Dep. Chem., Loyola Univ. Chicago, Chicago, IL, 60626,
USA
Organometallics (1991), 10(10), 3498-503
CODEN: ORGND7; ISSN: 0276-7333
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The isomerization of 2-(methyl-d3)-4-methyl-1,1,5,5-hexafluoro-3-penten-2-ol (I) into an equilibrium mixture of I and 2-methyl-4-(methyl-d3)-1,1,1,5,5-hexafluoro-3-penten-2-ol (II) in aqueous solution was studied by 1H and 2H NMR, under the Wacker conditions of low chloride (<1.0M) and acid (<0.5M) concns. The rate expression under these conditions was determined. The exchange of I with 18O-enriched water was studied by 13C NMR using isotope-induced shift methods and the rate of exchange was found to be the same as the rate of isomerization within exptl. error. This result requires that isomerization and exchange occur by a hydroxypalladation route, rather than through palladium(IV)- α -allyl intermediates. The rate expression for isomerization at low chloride concns. is identical with the rate expression for the Wacker oxidation of ethene to acetaldehyde.

This result is inconsistent with a proton inhibition arising from equilibrium hydroxypalladation but is consistent with proton loss from the Pd(II) coordination sphere in a preequil. step followed by a cis hydroxypalladation occurring from within the coordination sphere of the palladium(II). Stereochem. studies were conducted with chiral (E)-I. The observed result was the formation of chiral II with the opposite configuration of the initial I. This result is also consistent only with cis hydroxypalladation; so both kinetic and stereochem. mechanistic probes

give the same result.

IT 135708-35-9P 135708-36-OP 135708-37-1P

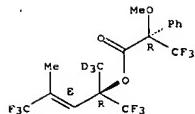
135708-38-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 135708-35-9 CAPLUS
CN Benzenesacetic acid, α -methoxy- α -(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(methyl-d3)-1-(trifluoromethyl)-2-butenoylester, [S-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

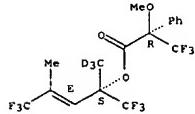
Absolute stereochemistry.
Double bond geometry as shown.

L4 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



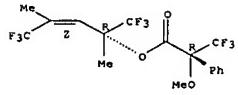
RN 135708-36-0 CAPLUS
CN Benzenesacetic acid, α -methoxy- α -(trifluoromethyl)-, 4,4,4-trifluoro-3-methyl-1-(methyl-d3)-1-(trifluoromethyl)-2-butenoylester, [S-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 135708-37-1 CAPLUS
CN Benzenesacetic acid, α -methoxy- α -(trifluoromethyl)-, 4,4,4-trifluoro-1,3-dimethyl-1-(trifluoromethyl)-2-butenoylester, [R-[R*,R*-(Z)]]- (9CI) (CA INDEX NAME)

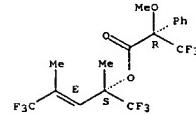
Absolute stereochemistry.
Double bond geometry as shown.



RN 135708-38-2 CAPLUS
CN Benzenesacetic acid, α -methoxy- α -(trifluoromethyl)-, 4,4,4-trifluoro-1,3-dimethyl-1-(trifluoromethyl)-2-butenoylester, [S-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

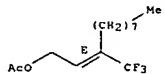
Absolute stereochemistry.
Double bond geometry as shown.

L4 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



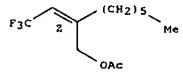
14 ANSWER 31 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1990:514701 CAPLUS
 DOCUMENT NUMBER: 113:114701
 TITLE: Trifluoromethylated allylic anion and radical; generation by the electronic inversion of π -allylic palladium complex by samarium diiodide
 AUTHOR(S): Hanzawa, Yuji; Ishizawa, Seiji; Kobayashi, Yoshiro; Taguchi, Takeo
 CORPORATE SOURCE: Tokyo Coll. Pharm., Hachioji, 192-03, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1990), 38(4), 1104-6
 CODEN: CPBTAL ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 113:114701
 AB Trifluoromethylated π -allylic Pd complexes were treated with Sm₂ to generate the trifluoromethylated allylic anion and radical species, which undergo reduction, elimination, or dimerization reactions. Treatment of PhCH₂CH₂CH(OAc)C(CF₃)₂:CH₂ with Pd(PPh₃)₄ and Sm₂ in the presence of MeCO(CH₂)₅Me gave 76% of a 4:3 isomeric mixture of adducts PhCH₂CH₂CH(C(CF₃)₂CH₂)Me(OH)(CH₂)₅Me.
 IT 120596-31-8 120596-33-0 129049-09-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with palladium tetrakis(triphenylphosphine) and samarium diiodide, allylic anion and radical species from)
 RN 120596-31-8 CAPLUS
 CN 2-Undecen-1-ol, 3-(trifluoromethyl)-, acetate, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 120596-33-0 CAPLUS
 CN 1-Octanol, 2-(2,2,2-trifluoroethylidene)-, acetate, (Z)- (9CI) (CA INDEX NAME)

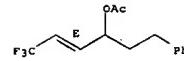
Double bond geometry as shown.



RN 129049-09-8 CAPLUS
 CN Benzenepropanol, α -(3,3,3-trifluoro-1-propenyl)-, acetate, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

14 ANSWER 31 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



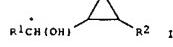
14 ANSWER 32 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1990:497086 CAPLUS
 DOCUMENT NUMBER: 113:97086
 TITLE: Preparation of optically active trifluoromethylhydroxycyclopropanes
 INVENTOR(S): Kitatsume, Tomoya; Takeda, Mitsunori
 PATENT ASSIGNEE(S): Kashima Oil Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 02049742 | A | 19900220 | JP 1988-200229 | 19880812 |
| JP 2642959 | B2 | 19970820 | | |

PRIORITY APPN. INFO.: JP 1988-200229 19880812

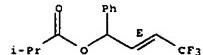
OTHER SOURCE(S): MARPAT 113:97086

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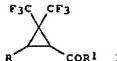
AB The title compds. (I; R₁, R₂ = C1-2 fluoroalkyl, C1-10 alkyl, C7-10 aralkyl, C6-10 aryl; provided that 2¹ of R₁, R₂ = C1-2 fluoroalkyl) of high optical purity, useful as intermediates for enzyme inhibitors, physiol. active substances, antitumor agents, and ferroelec. liquid crystals, were prepared. Thus, reduction of CF₃CH(OH)C₂H₅ with Na[AlH₂COC₂CH₂OMe]₂ in Et₂O followed by acetylation with AcCl in pyridine gave CF₃CH(OAc)CH₂Ph. Stereoselective hydrolysis of the latter with lipase MY in H₂O at 40-41° for 6.5 h gave (3S)-(E)-CF₃CH(OH)CH₂Ph (R₃ = Ac) and (3R)-(E)-CF₃CH(OH)CH₂CHPh (R₃ = H) (II). Carbone addition reaction of II with CH₂I₂ in the presence of Sm and HgCl₂ in THF at 0° for 1 h and room temperature for 2 h gave (1R)-(+)I (R₁ = CF₃, R₂ = Ph).
 IT 128726-32-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and carbene addition of, with methylene iodide)
 RN 128726-32-9 CAPLUS
 CN Propanoic acid, 2-methyl-, 4,4,4-trifluoro-1-phenyl-2-but enyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



10539639a.trn

14 ANSWER 33 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1989:1554137 CAPLUS
 DOCUMENT NUMBER: 111:154137
 TITLE: Synthesis of bis(trifluoromethyl) substituted
 pyrethroids
 AUTHOR(S): Mack, Helmut; Hanack, Michael
 CORPORATE SOURCE: Inst. Organische Chemie, Universitat Tubingen,
 Tubingen, D-7400, Fed. Rep. Ger.
 SOURCE: Liebigs Annalen der Chemie (1989), (9), 833-46
 CODEN: LACHDL ISSN: 0170-2041
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 111:154137
 GI

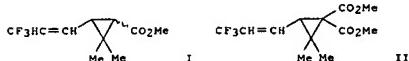


AB RCH:C(CF3)2 [R = CH:CCl2, CH:Me2, CH(OEt)2], were prepared from RCHO, C12C(CF3)2 and PPh3 and converted into 2,2-bis(trifluoromethyl)cyclopropanecarboxylates I [R1 = OEt] by reaction with Me2S+C-HCO2Et. I [R = CHO, R1 = OEt], obtained from (EtO)2CHCH:C(CF3)2 and Me2S+C-HCO2Et, is an important intermediate in the preparation of the bis(trifluoromethyl)-substituted pyrethroids I [R = CH:CH2, CH:CCl(CF3)2, CH:CCl(CF3); R1 = OEt]. Hydrolysis of I [R = CH:CCl2, CHClCHMe2; R1 = OEt] gave I [R1 = OH], which were converted to pyrethroid esters I [R1 = OCH(CN)C6H4OPh-3] via I [R1 = Cl]. 4-C1C6H4CH:C(CF3)2 reacts with Me2C(CN)OH to form 4-C1C6H4CH(CN)CH(CF3)2, prepared from the nitrile via the acid, was treated with 3-PhOC6H4CH(CN)OH to give hexafluoroenvalerate, 4-C1C6H4CH(CN)CH(CF3)2CO2CH(CN)C6H4OPh-3.

IT 121618-14-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclopropanation of, with ethoxycarbonylmethylenedimethylesulfurane)

RN 121618-14-2 CAPLUS
 CN 4-Hexen-3-ol, 6,6,6-trifluoro-2-methyl-5-(trifluoromethyl)-, acetate (9CI) (CA INDEX NAME)

14 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1989:212158 CAPLUS
 DOCUMENT NUMBER: 110:212158
 TITLE: Palladium(0)-catalyzed reactions of trifluoromethylated allylic ester derivatives: synthesis of trifluoromethylated chrysanthemic acid esters
 AUTHOR(S): Hanazawa, Yuji; Ishizawa, Seiji; Kobayashi, Yoshiro
 CORPORATE SOURCE: Tokyo Coll. Pharm., Hachioji, 192-03, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(10), 4209-12
 CODEN: CPBTAL ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 110:212158
 GI

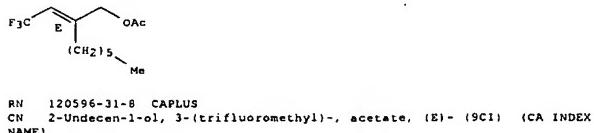


AB Reactions of RCH(OAc)CR1:CR2CF3 (R = PhCH2CH2, H; R1 = hexyl, N; R2 = octyl, H, PhCH2CH2CH(OAc)C(CF3):CH2 and CF3CH(OR1)CH:CR4R5 [R3 = Ac, CO2Et, P(O)(OEt)2, SO2C6H4Me-4; R4, R5 = H, hexyl] with NaCH(CO2Me)2 in the presence of palladium catalyst, e.g., (Ph3P)4Pd, and their use in synthesizing trifluoromethylated chrysanthemic acids I are described. Thus, CF3CH(OR1)CH:CHMe2OAc heated with NaCH(CO2Me)2 in THF in the presence of (Ph3P)4Pd to give CF3CH(OR1)CH:CHMe2CH(CO2Me)2, which was treated with DBU in the presence of bis(1,2-bis(diphenylphosphino)ethane)palladium to give 73% cyclopropanecarboxylate II. Treating II with NaCN in Me2SO gave 47% I.

IT 120596-30-7 120596-31-8 120596-32-9
 120596-33-0 120596-34-1 120449-09-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, with malonate in presence of palladium)

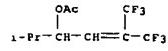
RN 120596-30-7 CAPLUS
 CN 1-Octanol, 2-(2,2,2-trifluoroethylidene)-, acetate, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



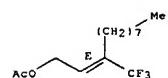
10539639a.trn

14 ANSWER 33 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



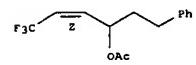
14 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.



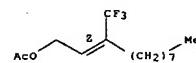
RN 120596-32-9 CAPLUS
 CN Benzenepropanol, α -(3,3,3-trifluoro-1-propenyl)-, acetate, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



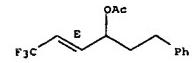
RN 120596-33-0 CAPLUS
 CN 1-Octanol, 2-(2,2,2-trifluoroethylidene)-, acetate, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 120596-34-1 CAPLUS
 CN 2-Undecen-1-ol, 3-(trifluoromethyl)-, acetate, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

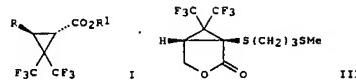


RN 120596-31-8 CAPLUS
 CN Benzenepropanol, α -(3,3,3-trifluoro-1-propenyl)-, acetate, (E)- (9CI) (CA INDEX NAME)

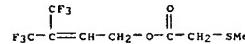
Double bond geometry as shown.

14 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 35 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1986:423961 CAPLUS
 DOCUMENT NUMBER: 105:23961
 TITLE: Stereoselective synthesis of gem-bis(trifluoromethyl)cyclopropane derivatives
 AUTHOR(S): Taguchi, Takeo; Hosoda, Akihiko; Torisawa, Yutaka;
 Shimazaki, Akinori; Kobayashi, Yoshiro; Tsushima,
 Kazunori
 CORPORATE SOURCE: Tokyo Coll. Pharm., Hachioji, 192-03, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(9),
 4085-7
 DOCUMENT TYPE: CODEN: CPBTAL; ISSN: 0009-2363
 LANGUAGE: Journal
 OTHER SOURCE(S): English
 CASREACT 105:23961
 GI

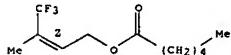


AB The trans-bis(trifluoromethyl)cyclopropanecarboxylate I (R = CH2OBz, R1 = Et) (II) was prepared in 44% yield by treating (CF3)2C:CHR with Me2S-C-HCO2Et. II was further converted to I (R = CH:CCl2; R1 = (NC)CHC6H4OPh-3) in 8 steps. The cis-derivative III was prepared in 43% yield by treating (CF3)2C:CHCH2O2CCH(SR2)2 [R22 = (CH2)3] with CF3SO3Me followed by KF and 18-crown-6 in CH2Cl2-DMF.
 IT 102710-53-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation and reaction of, with benzenethiol)
 RN 102710-53-2 CAPLUS
 CN Acetic acid, (methylthio)-, 4,4,4-trifluoro-3-(trifluoromethyl)-2-butenyl ester (9CI) (CA INDEX NAME)

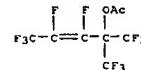


14 ANSWER 36 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1985:57745 CAPLUS
 DOCUMENT NUMBER: 102:57745
 TITLE: Design of novel insect anti-juvenile hormones:
 allylic alcohol derivatives
 AUTHOR(S): Quistad, Gary B.; Cerf, David C.; Kramer, Steven J.;
 Bergot, B. John; Schooley, David A.
 CORPORATE SOURCE: Dep. Biochem. Insect Res., Zocon Corp., Palo Alto,
 CA, 94304, USA
 SOURCE: Journal of Agricultural and Food Chemistry (1985),
 33(1), 47-50
 CODEN: JAFCAU; ISSN: 0021-8561
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Three analogs of 3,3-dimethyl-2-propenol (dimethylallyl alc.) were synthesized and found to possess anti-juvenile hormone activity when assayed on lepidopteran species (particularly the tobacco hornworm, Manduca sexta). The most active compound of those described, 3,3-dichloro-2-propenyl hexanoate (93404-30-9), caused precocious metamorphosis, inhibited juvenile hormone (JH) biosynthesis in vitro, and reduced JH titers in vivo.
 IT 93404-31-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and anti-juvenile hormone activity of)
 RN 93404-31-0 CAPLUS
 CN Hexanoic acid, 4,4,4-trifluoro-3-methyl-2-butenoylester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 37 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1971:517925 CAPLUS
 DOCUMENT NUMBER: 75:117925
 TITLE: Preparation and reactions of some carbinols
 containing the pentafluoropropenyl group
 AUTHOR(S): Tarrant, Paul; Whitfield, Ralph W., Jr.: Summerville,
 Richard H.
 CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL, USA
 SOURCE: Journal of Fluorine Chemistry (1971), 1(1), 31-40
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 1,1,1,2,3,3-Hexafluoropropane was dehydrofluorinated to yield a 1:1 mixture of (Z)- and (E)-1H-pentafluoropropene. This mixture reacted with BuLi to give (Z)-(pentafluoropropenyl)lithium, which reacted with carbonyl compounds to give exclusively (Z)-pentafluoropropenyl carbinols. The yields were greater than 50%, indicating that the lithium reagent does not retain its stereochem. identity at low temperature, contrary to the hydrocarbon analog. Hydrolysis of CF3CF:CFLi also gave exclusively the (Z)-fluorolefin. Treating (Z)-CF3CF:CF(CF3)2OH with SF4 gave the E isomer. Chemical properties of the carbinols are described.
 IT 33683-43-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 33683-43-1 CAPLUS
 CN 3-Penten-2-ol, 1,1,1,3,4,5,5,5-octafluoro-2-(trifluoromethyl)-, acetate (8CI) (CA INDEX NAME)



L4 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:58379 CAPLUS

DOCUMENT NUMBER: 70:58379

TITLE: Perfluorocalkyl and α -chloroperfluoroalkyl-3-acyloxy-1,3-butadienes and polymers

INVENTOR(S): Middleton, William J.

PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co.

SOURCE: U.S., 3 pp.

DOCUMENT TYPE: patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| US 3424732 | A | 19690128 | US 1965-509174 | 19651122 |
| PRIORITY APPLN. INFO.: | | | US 1965-509174 | A 19651122 |

AB (CF₃)₂C(OAc)CH₂:CH₂ (I) is prepared and pyrolyzed to give (CF₃)₂CHC(OAc):CH₂ (II) or a polymer of II. II is also polymerized with afree radical catalyst. The polymer melts at >220° and is suitable for molding into transparent film having good flexibility and excellent solvent resistance. Thus, MeC₆H₅COBND.CH 100, CF₃OCF₃ 100, and hydroquinone 1 g. was heated at 150° for 48 hrs. in a bomb to give 70.5 g. (CF₃)₂C(OH)CH₂:CH₂, b. 105-6°, nD₂₅ 1.3477, which [20.6 g.] was added slowly to 100 ml. MeOCH₂CH₂OMe containing 4.5 g. 54% NaH(in mineral oil). The mixture was cooled in an ice bath, treated slowly with 7.9 g. AcCl, and poured into 200 ml. water to give 22.2 g. I, b. 135-6°, nD₂₅ 1.3668, which (14 g.) was added during 1 hr. to a silica glass tube heated at 500° and inclined at 45°. The pyrolyze was distilled to give 8 g. II, b22 66-8°. II was polymerized at 60-90° in the presence of [Me₂C(CN)₂] or Bz₂O₂. I was also converted to the polymer of II by pyrolysis at 500° in a Pt tube followed by heating at 80-100°.

IT 20227-71-8P 28157-84-8P

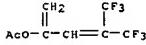
RL: PREP (Preparation)

(preparation of)

RN 20227-71-8 CAPLUS

CN 1,3-Pentadien-2-ol, 5,5,5-trifluoro-4-(trifluoromethyl)-, acetate (8CI)

(CA INDEX NAME)

RN 28157-84-8 CAPLUS
CN 1,3-Pentadien-2-ol, 5,5,5-trifluoro-4-(trifluoromethyl)-, acetate, polymers (8CI) (CA INDEX NAME)

CM 1

L4 ANSWER 39 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1968:86600 CAPLUS

DOCUMENT NUMBER: 68:86600

TITLE: Rearrangement of esters in the gas phase. II. Substituent effects on the rate of isomerization of allylic esters

AUTHOR(S): Lewis, Edward Sheldon; Hill, James Theo; Newman, Edward R.

CORPORATE SOURCE: Rice Univ., Houston, TX, USA

SOURCE: Journal of the American Chemical Society (1968), 90(3), 662-8

DOCUMENT TYPE: CODEN: JACSAT; ISSN: 0002-7863

LANGUAGE: Journal

CM 1

AB The rearrangement of α - and γ -trifluoromethylallyl trifluoroacetates, allyl- α -d2 trifluoroacetate, allyl trifluoroacetate-180, α , β -dimethylallyl acetate, and α , γ -dimethylallyl acetate was studied. In some cases a minor but detectable rearrangement to cis- as well as trans- γ -substituted allyl derivs. was observed. The rate of rearrangement of allyl acetate was within exptl. error the same whether followed by D or 180 labeling. The results were consistent with a transition state with carbonium carboxylate character. 21 references.

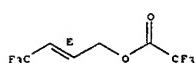
IT 19235-03-1 19235-04-2

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (rearrangement of, kinetics of)

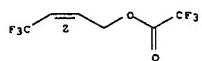
RN 19235-03-1 CAPLUS

CN Acetic acid, trifluoro-, 4,4,4-trifluoro-2-butenyl ester, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 19235-04-2 CAPLUS
CN Acetic acid, trifluoro-, 4,4,4-trifluoro-2-butenyl ester, (Z)- (8CI) (CA INDEX NAME)

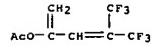
Double bond geometry as shown.



L4 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ACCESSION NUMBER: 1969:20227-71-8

DOCUMENT NUMBER: CMF CB H6 F6 O2



L4 ANSWER 40 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:490634 CAPLUS

DOCUMENT NUMBER: 65:90634

ORIGINAL REFERENCE NO.: 65:16962f-g Addition reactions of nitroso groups. Diene syntheses of nitrosobenzenes with 2-substituted 1,3-butadienes

AUTHOR(S): Kresze, G.; Korpiun, O.

CORPORATE SOURCE: Tech. Hochsch., Munich, Germany

SOURCE: Tetrahedron (1966), 22(8), 2493-504

DOCUMENT TYPE: CODEN: TETRAB; ISSN: 0040-4020

Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 65:90634

GI For diagram(s), see printed CA Issue.

AB Nitrosobenzenes add to 2-substituted butadienes to give, in most cases, 4-substituted 3,6-dihydro-1,2-oxazines (I). The structure of these adducts is proved by N.M.R. spectroscopy and chemical means. The

kinetics of the Diels-Alder reaction of 2-arylbutadienes with p-chloronitrosobenzene was studied.

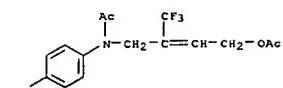
IT 7624-71-7P, Acetanilide, 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]-, acetate 7624-73-9P, Acetanilide, 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]-, trifluoroacetate

RL: PREP (Preparation)

(preparation of)

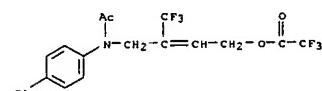
RN 7624-71-7 CAPLUS

CN Acetanilide, 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]-, acetate (7CI, 8CI) (CA INDEX NAME)



RN 7624-73-9 CAPLUS

CN Acetic acid, trifluoro-, ester with 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]acetanilide (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 41 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:490633 CAPLUS

DOCUMENT NUMBER: 65:90633

ORIGINAL REFERENCE NO.: 65:16962d-f

TITLE: Amino alcohols. XXIV. 4-Methyl- and

4-cyclohexylmorpholine-2,4-dione

AUTHOR(S): Drefahl, Guenther; Hartmann, Manfred; Skurk, Axel

CORPORATE SOURCE: Univ. Jena, Germany

SOURCE: Chemische Berichte (1966), 99(8), 2716-17

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 65:90633

AB cf. CA 64, 19600c; 65, 10472e. $H_2NCH_2CH_2OH$ (30.5 g.) added dropwise at 0° with stirring to 270 cc. $(CO_2Et)_2$ in 50 cc. EtOH yielded 42% $HOC_2CH_2NHCO_2Et$, b0.001 155-60°, n_D 1.4724. The distillation residue recrystd. from EtOH gave an amorphous, polymeric oxamic acid ester, m. 155-60°. $BzCH_2CH_2NH_2\cdot HBr$ (41 g.) in 100 cc. absolute EtOH was treated at 0° with 50 cc. 4N aq. KOH, filtered, and added dropwise to 135 cc. $(CO_2Et)_2$ in 50 cc. EtOH to give 44% $BzCH_2CH_2NHCO_2Et$, m. 56° (C6H6). $MnH_2CH_2CH_2OH$ (40 g.) in 100 cc. EtOH added dropwise at $0-5^\circ$. $(CO_2Et)_2$ in 20 cc. EtOH and refluxed 10 min. yielded 37% 4-methylmorpholine-2,3-dione (I), m. 98-9° (C6H6). The filtrate gave 30% $HOC_2CH_2NHCO_2Et$, b0.18 102-6°, n_D 1.7458. A mixture of 3.6 g. 2-cyclohexylamineethanol in 10 cc. EtOH and 5 cc.

$(CO_2Et)_2$ was refluxed 0.5 hr. to yield 84% 4-cyclohexyl analog of I, m. 123-3.5° (MePh).

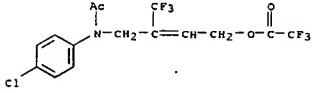
IT 7624-73-9; Acetic acid, trifluoro-, ester with 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butenyl]acetanilide

RL: PREP (Preparation)

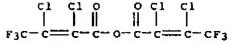
(preparation of)

RN 7624-73-9 CAPLUS

CN Acetic acid, trifluoro-, ester with 4'-chloro-N-[4-hydroxy-2-(trifluoromethyl)-2-butene]acetanilide (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 42 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 42 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1959:56049 CAPLUS

DOCUMENT NUMBER: 53:56049

ORIGINAL REFERENCE NO.: 53:10039f-i, 10040a

TITLE: Dichlorotri(trifluorocrotonic acid

INVENTOR(S): Baranuckas, Charles F.; Ashton, Wm. E.

PATENT ASSIGNEE(S): Hooker Chemical Corp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|-------------------|---|-----------------|----------|
| US 2863906 | ----- | 19581209 | US 1955-516304 | 19550617 |
| AB CF3CCl:CCClC13 | (C.A. 52, 14649a) | and 1567 g. H ₂ SO ₄ heated | | |
| at 130° 10 hrs., cooled and 500 ml. H ₂ O added. The lower layer was extracted with 10% NaOH solution. Addition of excess HCl, extraction with Et ₂ O, and | | | | |
| distillation gave 780 g. CF3CCl:CClCO ₂ H (I), b11 83-5°; 81 g. I was obtained from the H ₂ SO ₄ layer. Addition of 391 g. PhCCl ₃ to 313.5 g. I | | | | |
| at 135° followed by 0.5 hr. at 170° gave 281 g. CF3CCl:CClCOCl (II), b. 113-15°. Distillation of 104.5 g. I from 71 g. P2O ₅ and redistn. from 15 g. ROH gave 55 g. (CF3CCl:CClCO ₂ H, b11 103-4°. II and ROH gave the following esters (R, b.p./mm., n _D and % yield given): Me, 141-3°/743, 1.4103, 71; Et, 155-6°/742, 1.4108, 76; Bu, 193°/746, 1.4188, 60; Am, 207-10°/746, 1.4221, 89; n-C ₈ H ₁₇ , 134°/13, 1.4310, 50; iso-Pr, 165°/760, 1.4097, 82; CF ₃ CH ₂ , 145-6°/735, 1.3780, 82; tert-Bu, 65-6°/12, 1.4122, 30; CH ₂ :CHCH ₂ , 170-2°/760, 1.4264, 43; tetrahydrofuryl, 143-5°/30, 1.4457, 55; Ph, 113-15°/13, 1.4832, 49; cyclohexyl, 75-7°/2.5, 1.4468, 68; methylcyclohexyl, 79-81°/2.2, 1.4460, 46; -CH ₂ CH ₂ -, 163-4°/22, 1.4410, 81; -CH ₂ CHMe-, 159°/13, 1.4396, 56; -(CH ₂) ₄ -, 148-56°/3, 1.4439, 42; -CH ₂ CH ₂ COCH ₂ -, 189-90°/13, 1.4446, 43. Amines and II gave amides (amine, b.p./mm., and n _D of amide given): NH ₃ (III), -, - (m. 123-5°); BuNH ₂ , 167-8°/30, 1.4465; PhCH ₂ CH ₂ NH ₂ , -, - (m. 97-8°); (Me ₂ CH) ₂ NH, 134-6°/26, 1.4462; Bu ₂ NH, -, - (m. 14510; PhNH ₂ , -, - (m. 102-8°); H ₂ NC ₂ CH ₂ CH ₂ NH ₂ , -, - (m. 241-2°). Distillation of 31.2 g. III from 42.6 g. P2O ₅ at mild vacuum gave 11.5 g. CF3CCl:CClCN, b. 107-8°. I and esters are useful as anthelmintic agents. Salts prepared by evaporation of solns. of I and metal carbonates are useful as grease thickeners. Amides are insect repellents. | | | | |
| IT 654-24-0, Crotonic acid, 2,3-dichloro-4,4,4-trifluoro-, anhydride (and esters) | | | | |
| RN 654-24-0 CAPLUS | | | | |
| CN 2-Butenoic acid, 2,3-dichloro-4,4,4-trifluoro-, anhydride (9CI) (CA INDEX NAME) | | | | |

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| => log Y | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 222.28 | 395.51 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -32.76 | -32.76 |

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